```
=> s l1 full
FULL SEARCH INITIATED 11:16:52 FILE 'CASREACT'
SCREENING COMPLETE -     6095 REACTIONS TO VERIFY FROM      502 DOCUMENTS

100.0% DONE    6095 VERIFIED    1458 HIT RXNS (   120 INCOMP)     114 DOCS
SEARCH TIME: 00.00.04

L3          114 SEA SSS FUL L1 (  1458 REACTIONS)

=> s l3 and carbon monoxide
         50134 CARBON
          1717 CARBONS
         51225 CARBON
                 (CARBON OR CARBONS)
          6370 MONOXIDE
            92 MONOXIDES
          6411 MONOXIDE
                 (MONOXIDE OR MONOXIDES)
          5849 CARBON MONOXIDE
                 (CARBON(W)MONOXIDE)
L4            0 L3 AND CARBON MONOXIDE

=> s carbon monoxide
         50134 CARBON
          1717 CARBONS
         51225 CARBON
                 (CARBON OR CARBONS)
          6370 MONOXIDE
            92 MONOXIDES
          6411 MONOXIDE
                 (MONOXIDE OR MONOXIDES)
L5        5849 CARBON MONOXIDE
                 (CARBON(W)MONOXIDE)

=> file reg
FILE 'REGISTRY' ENTERED AT 11:17:25 ON 16 MAR 2009
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provided by InfoChem.

STRUCTURE FILE UPDATES:   13 MAR 2009  HIGHEST RN 1120564-02-4
DICTIONARY FILE UPDATES:  13 MAR 2009  HIGHEST RN 1120564-02-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html
```

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```
=> s carbon monoxide/cn
L6            1 CARBON MONOXIDE/CN

=> d rsd

L6   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2009 ACS on STN


=> d rn

L6   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2009 ACS on STN
RN   630-08-0  REGISTRY


=> file casreact
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FILE CONTENT:1840 - 15 Mar 2009 VOL 150 ISS 12

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*************************************************************
*                                                           *
*     CASREACT now has more than 16.5 million reactions     *
*                                                           *
*************************************************************

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This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> s 630-08-0
L7        10878 630-08-0

=> d his

     (FILE 'HOME' ENTERED AT 11:15:49 ON 16 MAR 2009)

     FILE 'CASREACT' ENTERED AT 11:16:04 ON 16 MAR 2009
L1                STRUCTURE UPLOADED
L2              3 S L1
L3            114 S L1 FULL
L4              0 S L3 AND CARBON MONOXIDE
L5           5849 S CARBON MONOXIDE
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FILE 'REGISTRY' ENTERED AT 11:17:25 ON 16 MAR 2009
L6 1 S CARBON MONOXIDE/CN

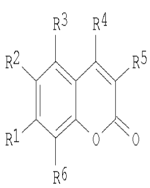
FILE 'CASREACT' ENTERED AT 11:17:52 ON 16 MAR 2009
L7 10878 S 630-08-0

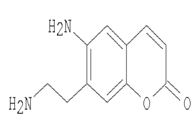
=> s l7 and l3
L8 2 L7 AND L3

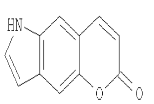
=> d cbib abs crd 1-
YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/(N):y

L8 ANSWER 1 OF 2 CASREACT COPYRIGHT 2009 ACS on STN
144:292572 Diaminocoumarins as fluorogenic substrates for monoamine oxidases, and their preparation, pharmaceutical compositions, photophysical properties, and a method for detecting active monoamine oxidases and their inhibitors for treatment of nervous system disorders. Chen, Gong; Yee, Dominic J.; Gubernator, Niko; Sames, Dalibor (The Trustees of Columbia University in the City of New York, USA). PCT Int. Appl. WO 2006026368 A2 20060309, 278 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IS, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2005-US30276 20050825. PRIORITY: US 2004-604538P 20040825.

GI


I


II


III

AB The invention relates to compds. of formula I, which are useful for detecting the activity of monoamine oxidases (MAO), compds. useful for competitively inhibiting monoamine oxidases, for determining inhibitors of monoamine oxidases and compds. useful for treating monoamine

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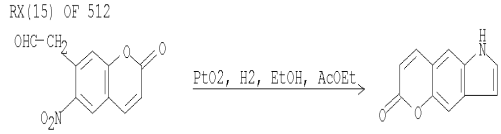
oxidase-related nervous system pathologies, as well as pharmaceutical compns. and methods of manufacture thereof. Compds. of formula I wherein R1 is H, alkyl, alkenyl, alkynyl, (un)substituted (hetero)aryl, cycloalkyl, NH2 and derivs., alkyl-CO2H, alkyl-OH, alkyl-NH2, halo, CX3, or indole; R2-R6 are independently H, OH, alkyl, alkenyl, alkynyl, (un)substituted (hetero)aryl, cycloalkyl, NH2 and derivs., alkyl-CO2H, alkyl-OH, alkyl-NH2, O-alkyl, O-alkenyl, O-alkynyl, O-aryl, O-cycloalkyl, CX3, halo, or indole; R1R2 and R1R6 may independently form an unsubstituted pyrrole; R1R2R6 may form an octahydroquinazolizine; R2R3 may form a pyrrole; X is halo; or pharmaceutically acceptable salts, or stereoisomers thereof are claimed in this invention. The process for preparing these fluorogenic substrates, and a method for identifying a test compound as a substrate of MAO are also claimed. Example compound II was prepared by nitration of 7-methylcoumarin, and the resulting 7-methyl-6-nitrocoumarin underwent condensation with DMF di-Me acetal to give the corresponding coumarin-enamine, which was hydrolyzed to give 7-(2-oxoethyl)-6-nitrocoumarin, which underwent reductive amination with dibenzosuberylamine; the resulting 7-(dibenzosuberylaminoethyl)-6-nitrocoumarin was reduced to the 6-aminocoumarin compound, which was hydrolyzed to give coumarin II. The invention compds. were evaluated for their photophys. properties and their enzymic activity toward MAO-A and MAO-B. Coumarin II showed λmax 352 nm, ε 2000±100 M-1cm-1, Φ 0.0017±0.0001, and λem was not detected. The invention compds. were evaluated for their ability to convert to the corresponding indole in the presence of MAO-A and MAO-B. Enzyme-catalyzed indole formation was realized after 24 h by reading fluorescence emission upon excitation at the absorbance maxima of the resp. indoles. Only diamino-coumarin II showed a significant conversion to its indole III in the presence of MAO-A and MAO-B. The enzyme kinetics for fluorogenic probe II were also determined Compound II showed for MAO-A: Km = 30.9±1.8 μM, Kcat = 0.475 min-1, Kcat/Km = 0.015 min-1 μM-1, Vmax(mitochondria) = 0.0570 nmol min-1 mg-1; and for MAO-B: Km = 510±40 μM, Kcat = 20.62 min-1, Kcat/Km = 0.040 min-1 μM-1, and Vmax(mitochondria) = 1.2 nmol min-1 mg-1. These results indicate that coumarin probe II is a good substrate for monoamine oxidase and could be useful as a fluorescent reporter for monoamine oxidase.

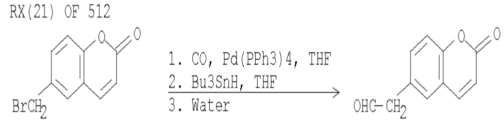
RX(15) OF 512



83%

CON: 2 hours, room temperature

RX(21) OF 512

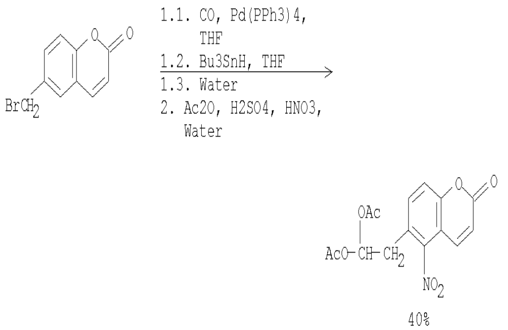


(step 1)

20%

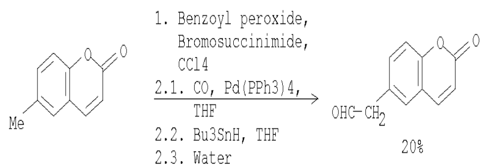
CON: STAGE(1) 50 deg C
STAGE(2) 2 hours, 50 deg C

RX(107) OF 512 - 2 STEPS



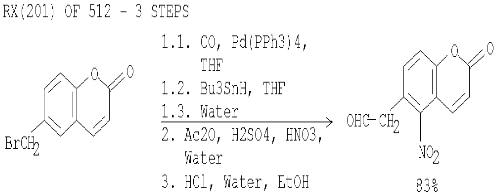
NOTE: 2) fuming nitric acid used
CON: STEP(1.1) 50 deg C
STEP(1.2) 2 hours, 50 deg C
STEP(2) 2 hours, 0 deg C

RX(181) OF 512 - 2 STEPS



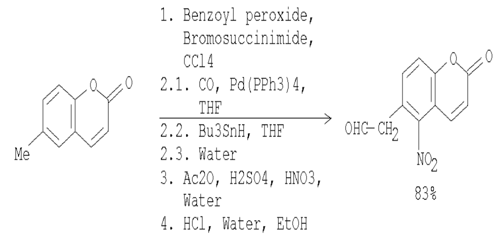
CON: STEP(1.1) room temperature; 12 hours, reflux
STEP(2.1) 50 deg C
STEP(2.2) 2 hours, 50 deg C

RX(201) OF 512 - 3 STEPS



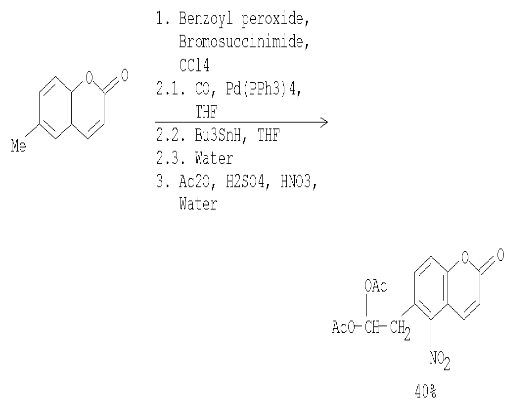
NOTE: 2) fuming nitric acid used
CON: STEP(1.1) 50 deg C
STEP(1.2) 2 hours, 50 deg C
STEP(2) 2 hours, 0 deg C
STEP(3) 1 hour, 110 deg C

RX(202) OF 512 - 4 STEPS



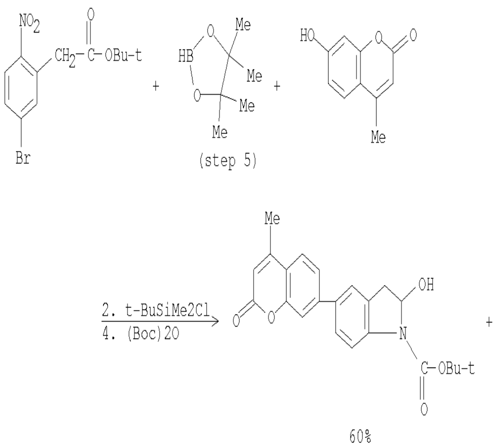
NOTE: 3) fuming nitric acid used
CON: STEP(1.1) room temperature; 12 hours, reflux
STEP(2.1) 50 deg C
STEP(2.2) 2 hours, 50 deg C
STEP(3) 2 hours, 0 deg C
STEP(4) 1 hour, 110 deg C

RX(317) OF 512 - 3 STEPS

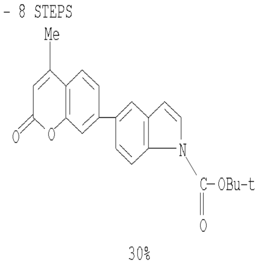


NOTE: 3) fuming nitric acid used
CON: STEP(1.1) room temperature; 12 hours, reflux
STEP(2.1) 50 deg C
STEP(2.2) 2 hours, 50 deg C
STEP(3) 2 hours, 0 deg C

RX(388) OF 512 - 8 STEPS

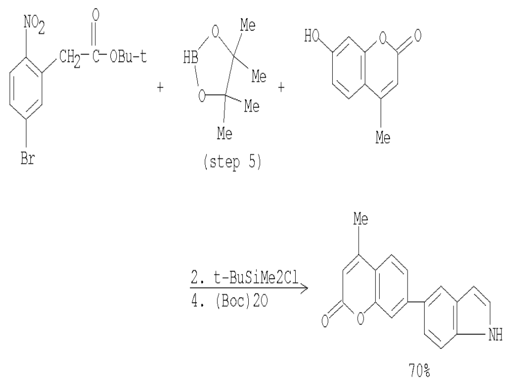


RX(388) OF 512 - 8 STEPS



NOTE: 6) Suzuki coupling in stage 2, key step in stage 2, 8)
      Dess-Martin oxidation
CON: STEP(1.1) 0 deg C; 1 hour, 0 deg C
      STEP(2.1) 0 deg C; overnight, room temperature
      STEP(3) 4 hours, room temperature
      STEP(4) 20 hours, reflux
      STEP(5) 4 hours, 100 deg C
      STEP(6.1) 2 hours, room temperature
      STEP(6.2) 20 hours, 80 deg C
      STEP(7.1) room temperature; 30 minutes, room temperature
      STEP(8.1) room temperature; 30 minutes, room temperature

RX(497) OF 512 - 9 STEPS



NOTE: 6) Suzuki coupling in stage 2, key step in stage 2, 8)
      Dess-Martin oxidation
CON: STEP(1.1) 0 deg C; 1 hour, 0 deg C
      STEP(2.1) 0 deg C; overnight, room temperature
      STEP(3) 4 hours, room temperature
      STEP(4) 20 hours, reflux
      STEP(5) 4 hours, 100 deg C
      STEP(6.1) 2 hours, room temperature
      STEP(6.2) 20 hours, 80 deg C
      STEP(7.1) room temperature; 30 minutes, room temperature
      STEP(8.1) room temperature; 30 minutes, room temperature
      STEP(9) 30 minutes, room temperature

L8   ANSWER 2 OF 2 CASREACT COPYRIGHT 2009 ACS on STN

142:411180 Synthesis of 5-Substituted-1H-indol-2-yl-1H-quinolin-2-ones: A Novel Class of KDR Kinase Inhibitors. Kuethe, Jeffrey T.; Wong, Audrey; Qu, Chuanxing; Smitrovich, Jacqueline; Davies, Ian W.; Hughes, David L. (Department of Process Research, Merck & Co., Inc., Rahway, NJ, 07065, USA). Journal of Organic Chemistry, 70(7), 2555-2567 (English) 2005. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

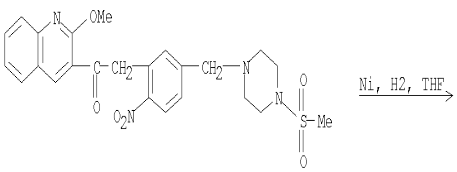
GI

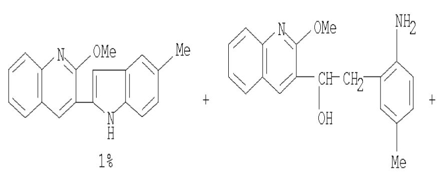
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB   A number of approaches for the synthesis of the 1H-indol-2-yl-1H-quinolin-2-one ring system found in the potent and selective KDR kinase inhibitor I are described. The preparation and reaction of trimethylsilylnitrobenzene II with 2-methoxy-3-quinolinecarboxaldehyde afforded alc. III, which was the key intermediate for the preparation of the target compds. Conversion of alc. III to either nitroketone IV or

nitrostyrene V set the stage for reductive cyclization. The quinolin-2-one functionality was unmasked in the last step to provide compound I in 56-60% overall yield from readily available starting materials.

RX(22) OF 350

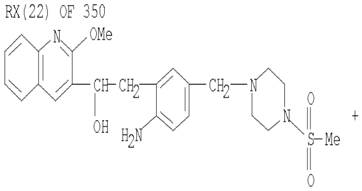




1%

1%

RX(22) OF 350



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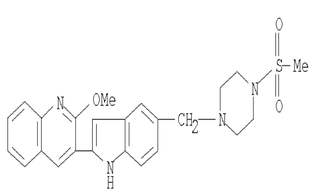

90%

NOTE: Raney Nickel used
CON: 7.5 hours, 65 deg C, 40 psi

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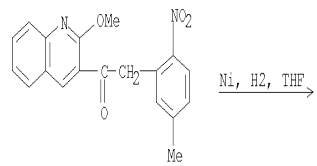
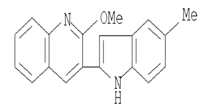
RX(27) OF 350

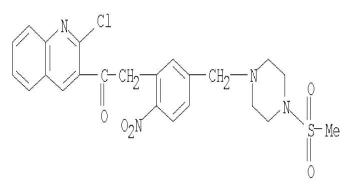


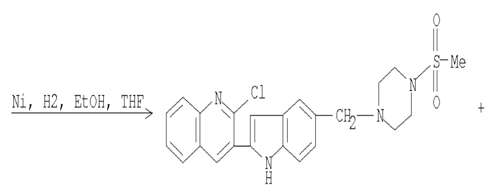


76%

NOTE: Raney Nickel used
CON: 7.5 hours, 65 deg C, 40 psi

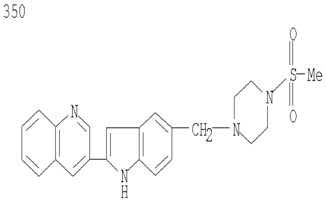
RX(28) OF 350





46%

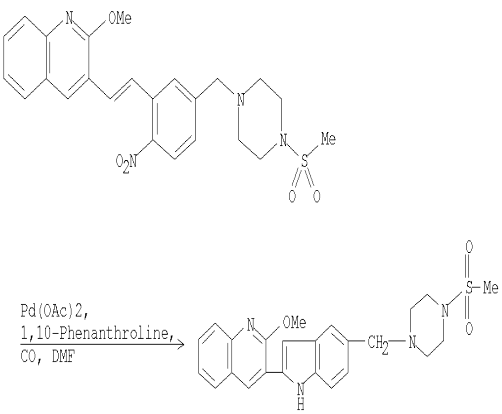
RX(28) OF 350



23%

NOTE: Raney Nickel used
CON: 20 hours, room temperature, 40 psi

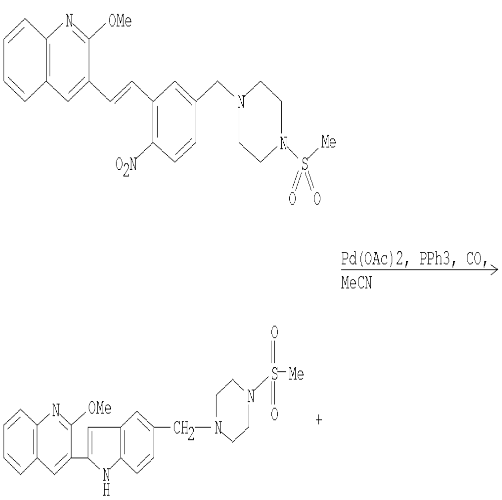
RX(36) OF 350



94%

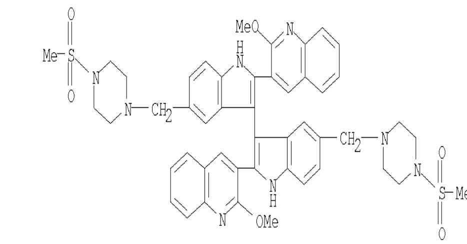
CON: 14 hours, 70 deg C, 15 psi

RX(37) OF 350



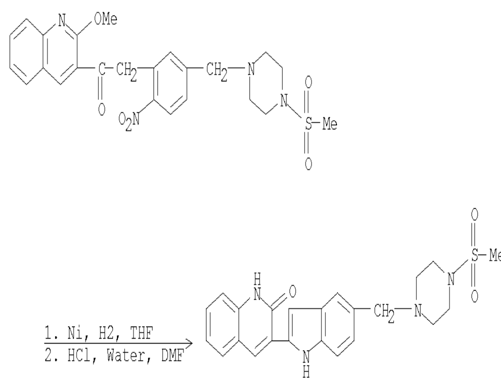
95%

RX(37) OF 350



CON: 15 hours, 70 deg C, 60 atm

RX(58) OF 350 - 2 STEPS



HCl

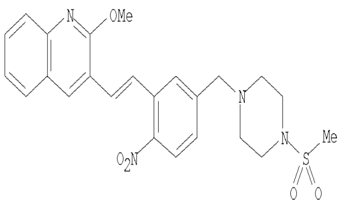
100%

NOTE: 1) Raney Nickel used

CON: STEP(1) 7.5 hours, 65 deg C, 40 psi

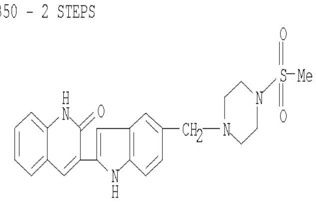
Print selected from 10562215.trn

RX(59) OF 350 - 2 STEPS



1. Pd(OAc)2,
   1,10-Phenanthroline,
   CO, DMF
2. HCl, Water, DMF

RX(59) OF 350 - 2 STEPS

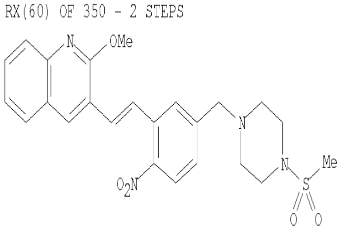


HCl

100%

CON: STEP(1) 14 hours, 70 deg C, 15 psi

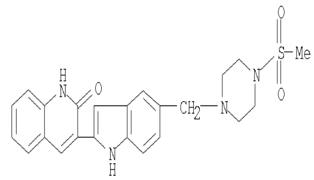
RX(60) OF 350 - 2 STEPS



1. Pd(OAc)2, PPh3, CO,
   MeCN
2. HCl, Water, DMF

Print selected from 10562215.trn

RX(60) OF 350 - 2 STEPS

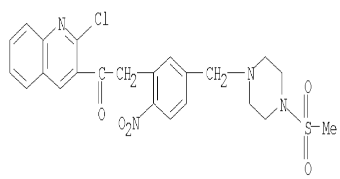


HCl

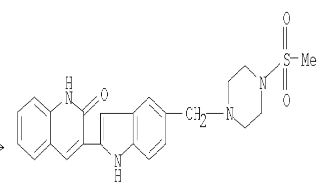
100%

CON: STEP(1) 15 hours, 70 deg C, 60 atm

RX(79) OF 350 - 2 STEPS



1. Ni, H2, EtOH, THF
2. AcOH, Water

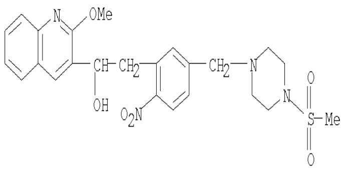


HCl

93%

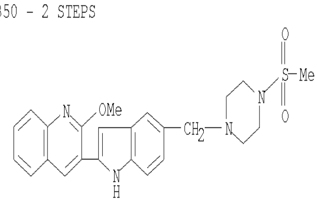
NOTE: 1) Raney Nickel used
CON: STEP(1) 20 hours, room temperature, 40 psi
      STEP(2) reflux

RX(81) OF 350 - 2 STEPS



1.1. $(CF3CO)2O$,
S:108-21-4
1.2. DBU
2. Pd(OAc)2,
1,10-Phenanthroline,
CO, DMF

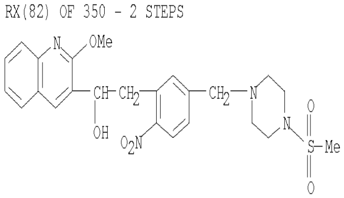
RX(81) OF 350 - 2 STEPS



94%

NOTE: 1) stereoselective
CON: STEP(1.1) 30 minutes, room temperature
STEP(1.2) 30 minutes, 60 deg C
STEP(2) 14 hours, 70 deg C, 15 psi

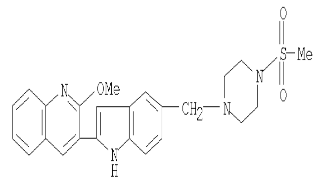
RX(82) OF 350 - 2 STEPS



1.1. $(CF3CO)2O$,
S:108-21-4
1.2. DBU
2. Pd(OAc)2, PPh3, CO,
MeCN

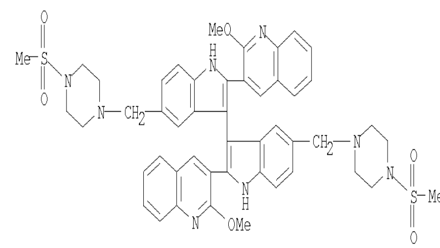
Print selected from 10562215.trn

RX(82) OF 350 - 2 STEPS



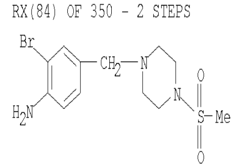
+

95%



NOTE: 1) stereoselective
CON: STEP(1.1) 30 minutes, room temperature
STEP(1.2) 30 minutes, 60 deg C
STEP(2) 15 hours, 70 deg C, 60 atm

RX(84) OF 350 - 2 STEPS



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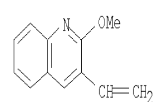
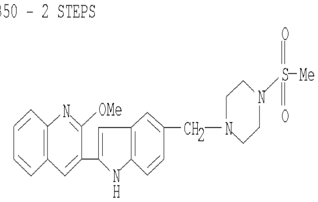


1. Tri-o-tolylphosphine,
Pd(OAc)2, Et3N,
DMF
2. Pd(OAc)2,
1,10-Phenanthroline,
CO, DMF

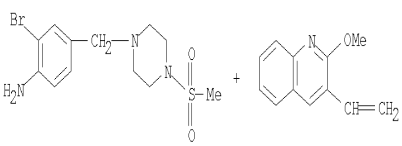
RX(84) OF 350 - 2 STEPS



94%

NOTE: 1) stereoselective
CON: STEP(1) 4 hours, 100 deg C
STEP(2) 14 hours, 70 deg C, 15 psi

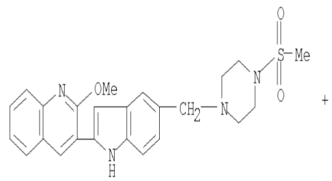
RX(85) OF 350 - 2 STEPS



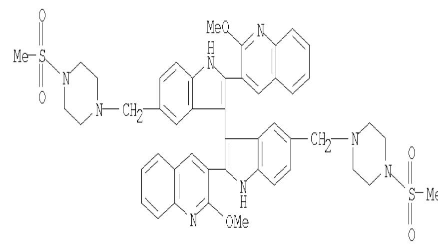
1. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
2. Pd(OAc)2, PPh3, CO, MeCN

Print selected from 10562215.trn

RX(85) OF 350 - 2 STEPS

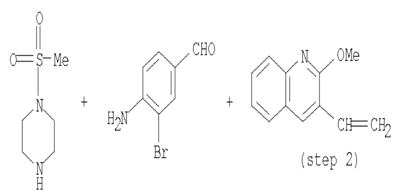


95%



NOTE: 1) stereoselective
CON: STEP(1) 4 hours, 100 deg C
STEP(2) 15 hours, 70 deg C, 60 atm

RX(115) OF 350 - 3 STEPS

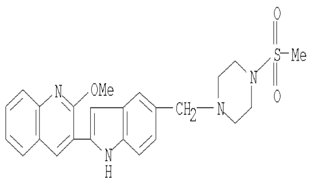


(step 2)

1.1. Na.(AcO)3BH, CH2Cl2
1.2. NH4Cl, Water
2. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
3. Pd(OAc)2, 1,10-Phenanthroline, CO, DMF

Print selected from 10562215.trn

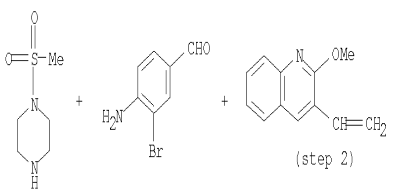
RX(115) OF 350 - 3 STEPS



94%

NOTE: 2) stereoselective
CON: STEP(1.1) 4 hours, room temperature
STEP(1.2) room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 14 hours, 70 deg C, 15 psi

RX(116) OF 350 - 3 STEPS

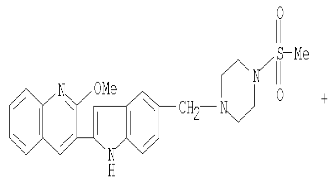


(step 2)

1.1. Na.(AcO)3BH, CH2Cl2
1.2. NH4Cl, Water
2. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
3. Pd(OAc)2, PPh3, CO, MeCN

Print selected from 10562215.trn

RX(116) OF 350 - 3 STEPS



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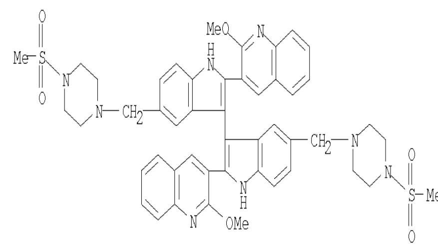
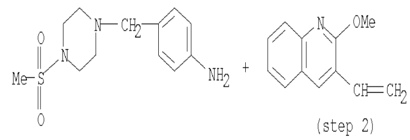


NOTE: 2) stereoselective
CON: STEP(1.1) 4 hours, room temperature
STEP(1.2) room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 15 hours, 70 deg C, 60 atm

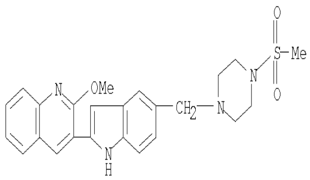
RX(122) OF 350 - 3 STEPS



(step 2)

1. C:98327-87-8, R:338746-12-6, KBr, Water, AcOH
2. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
3. Pd(OAc)2, 1,10-Phenanthroline, CO, DMF

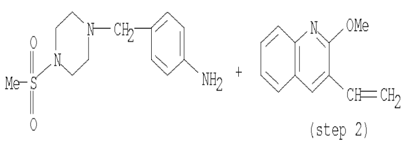
RX(122) OF 350 - 3 STEPS



94%

NOTE: 2) stereoselective
CON: STEP(1) 4 hours, room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 14 hours, 70 deg C, 15 psi

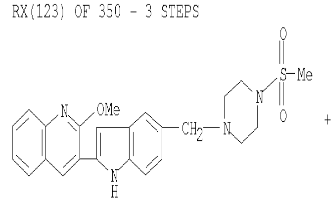
RX(123) OF 350 - 3 STEPS



(step 2)

1. C:98327-87-8, R:338746-12-6, KBr, Water, AcOH
2. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
3. Pd(OAc)2, PPh3, CO, MeCN

RX(123) OF 350 - 3 STEPS



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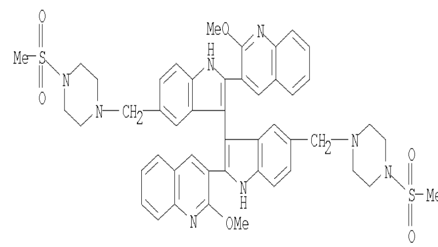
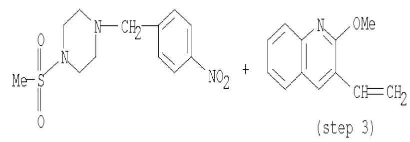


NOTE: 2) stereoselective
CON: STEP(1) 4 hours, room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 15 hours, 70 deg C, 60 atm

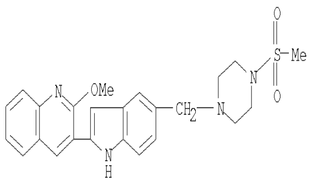
RX(129) OF 350 - 4 STEPS



(step 3)

1. Pd, H2, AcOEt
2. C:98327-87-8, R:338746-12-6, KBr, Water, AcOH
3. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
4. Pd(OAc)2, 1,10-Phenanthroline, CO, DMF

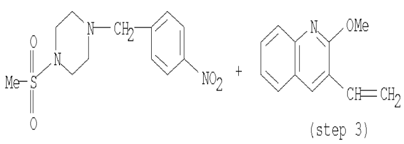
RX(129) OF 350 - 4 STEPS



94%

NOTE: 3) stereoselective
CON: STEP(1) 4 hours, room temperature
STEP(2) 4 hours, room temperature
STEP(3) 4 hours, 100 deg C
STEP(4) 14 hours, 70 deg C, 15 psi

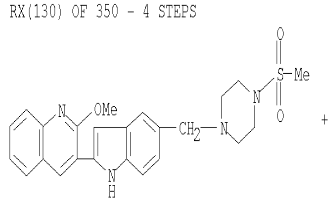
RX(130) OF 350 - 4 STEPS



(step 3)

1. Pd, H2, AcOEt
2. C:98327-87-8, R:338746-12-6, KBr, Water, AcOH
3. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
4. Pd(OAc)2, PPh3, CO, MeCN

RX(130) OF 350 - 4 STEPS



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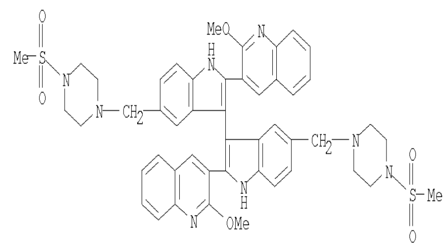
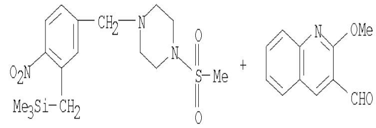


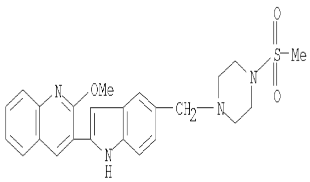
NOTE: 3) stereoselective
CON: STEP(1) 4 hours, room temperature
STEP(2) 4 hours, room temperature
STEP(3) 4 hours, 100 deg C
STEP(4) 15 hours, 70 deg C, 60 atm

RX(164) OF 350 - 3 STEPS



1. Bu4N.F, S:108-21-4
2.1. (CF3CO)2O, S:108-21-4
2.2. DBU
3. Pd(OAc)2, 1,10-Phenanthroline, CO, DMF

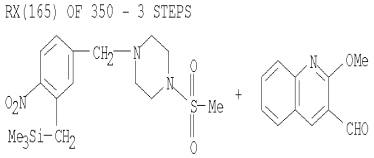
RX(164) OF 350 - 3 STEPS



94%

NOTE: 1) key intermediate, 2) stereoselective
CON: STEP(1.1) room temperature; 30 minutes, room temperature
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 30 minutes, 60 deg C
STEP(3) 14 hours, 70 deg C, 15 psi

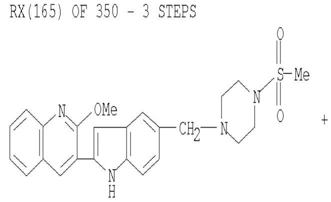
RX(165) OF 350 - 3 STEPS



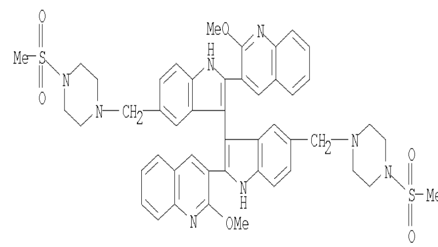
1. Bu4N.F, S:108-21-4
2.1. (CF3CO)2O,
S:108-21-4
2.2. DBU
3. Pd(OAc)2, PPh3, CO,
MeCN

Print selected from 10562215.trn

RX(165) OF 350 - 3 STEPS

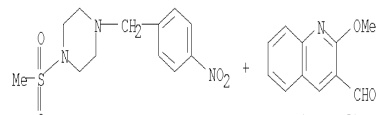


95%



NOTE: 1) key intermediate, 2) stereoselective
CON: STEP(1.1) room temperature; 30 minutes, room temperature
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 30 minutes, 60 deg C
STEP(3) 15 hours, 70 deg C, 60 atm

RX(168) OF 350 - 4 STEPS

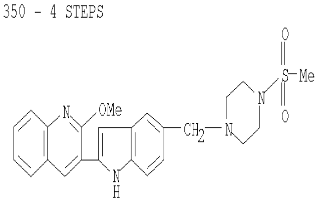


(step 2)

1.1. Me3SiCH2MgCl,
Et2O, THF
1.2. I2, Water
2. Bu4N.F, S:108-21-4
3.1. (CF3CO)2O,
S:108-21-4
3.2. DBU
4. Pd(OAc)2,
1,10-Phenanthroline,
CO, DMF

Print selected from 10562215.trn

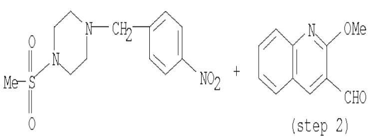
RX(168) OF 350 - 4 STEPS



94%

NOTE: 2) key intermediate, 3) stereoselective
CON: STEP(1.1) -20 deg C; <-5 deg C; 30 minutes, -20 deg C
STEP(1.2) 3 hours, room temperature
STEP(2.1) room temperature; 30 minutes, room temperature
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 30 minutes, 60 deg C
STEP(4) 14 hours, 70 deg C, 15 psi

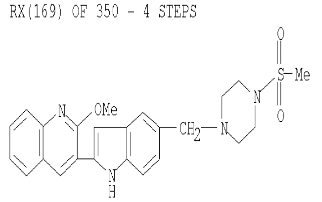
RX(169) OF 350 - 4 STEPS



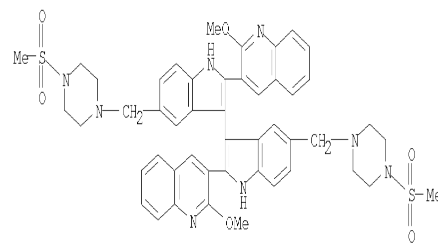
(step 2)

1.1. Me3SiCH2MgCl, Et2O, THF
1.2. I2, Water
2. Bu4N.F, S:108-21-4
3.1. (CF3CO)2O, S:108-21-4
3.2. DBU
4. Pd(OAc)2, PPh3, CO, MeCN
→

RX(169) OF 350 - 4 STEPS

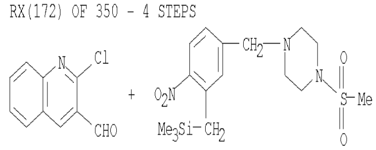


95%



NOTE: 2) key intermediate, 3) stereoselective
CON: STEP(1.1) -20 deg C; <-5 deg C; 30 minutes, -20 deg C
STEP(1.2) 3 hours, room temperature
STEP(2.1) room temperature; 30 minutes, room temperature
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 30 minutes, 60 deg C
STEP(4) 15 hours, 70 deg C, 60 atm

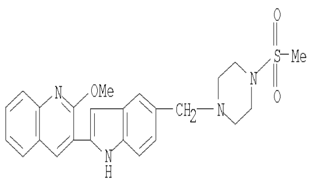
RX(172) OF 350 - 4 STEPS



(step 2)

1. MeOH, KOH
2. Bu4N.F, S:108-21-4
3.1. (CF3CO)2O, S:108-21-4
3.2. DBU
4. Pd(OAc)2, 1,10-Phenanthroline, CO, DMF
→

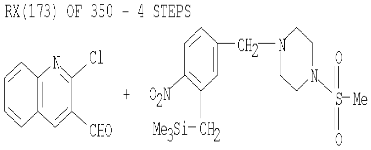
RX(172) OF 350 - 4 STEPS



94%

NOTE: 2) key intermediate, 3) stereoselective
CON: STEP(1) 2.5 hours, reflux
STEP(2.1) room temperature; 30 minutes, room temperature
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 30 minutes, 60 deg C
STEP(4) 14 hours, 70 deg C, 15 psi

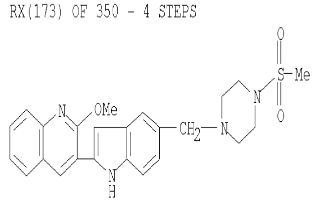
RX(173) OF 350 - 4 STEPS



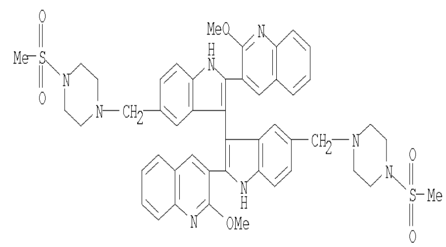
(step 2)

1. MeOH, KOH
2. Bu4N.F, S:108-21-4
3.1. (CF3CO)2O, S:108-21-4
3.2. DBU
4. Pd(OAc)2, PPh3, CO, MeCN

RX(173) OF 350 - 4 STEPS

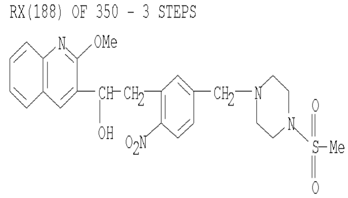


95%



NOTE: 2) key intermediate, 3) stereoselective
CON: STEP(1) 2.5 hours, reflux
STEP(2.1) room temperature; 30 minutes, room temperature
STEP(3.1) 30 minutes, room temperature
STEP(3.2) 30 minutes, 60 deg C
STEP(4) 15 hours, 70 deg C, 60 atm

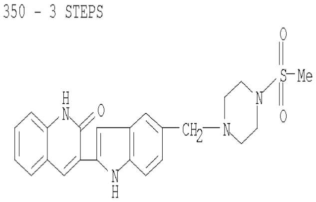
RX(188) OF 350 - 3 STEPS



1.1. (CF3CO)2O, S:108-21-4
1.2. DBU
2. Pd(OAc)2, 1,10-Phenanthroline, CO, DMF
3. HCl, Water, DMF

Print selected from 10562215.trn

RX(188) OF 350 - 3 STEPS

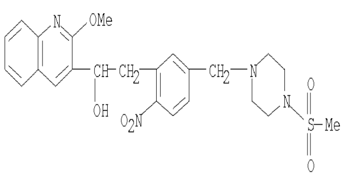


HCl

100%

NOTE: 1) stereoselective
CON: STEP(1.1) 30 minutes, room temperature
STEP(1.2) 30 minutes, 60 deg C
STEP(2) 14 hours, 70 deg C, 15 psi

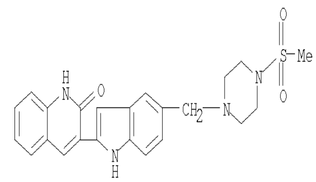
RX(189) OF 350 - 3 STEPS



1.1. (CF3CO)2O,
S:108-21-4
1.2. DBU
2. Pd(OAc)2, PPh3, CO,
MeCN
3. HCl, Water, DMF

Print selected from 10562215.trn

RX(189) OF 350 - 3 STEPS

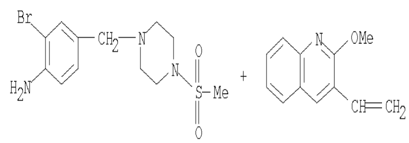


HCl

100%

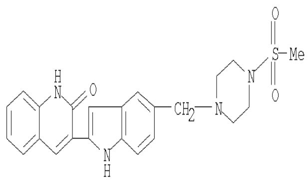
NOTE: 1) stereoselective
CON: STEP(1.1) 30 minutes, room temperature
STEP(1.2) 30 minutes, 60 deg C
STEP(2) 15 hours, 70 deg C, 60 atm

RX(190) OF 350 - 3 STEPS



1. Tri-o-tolylphosphine,
Pd(OAc)2, Et3N,
DMF
2. Pd(OAc)2,
1,10-Phenanthroline,
CO, DMF
3. HCl, Water, DMF

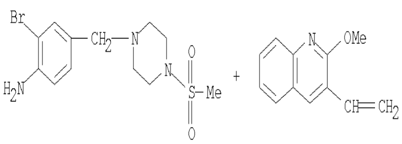
RX(190) OF 350 - 3 STEPS



HCl
100%

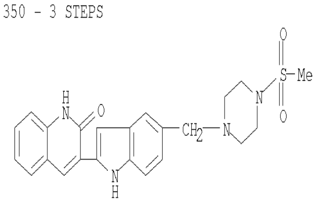
NOTE: 1) stereoselective
CON: STEP(1) 4 hours, 100 deg C
STEP(2) 14 hours, 70 deg C, 15 psi

RX(191) OF 350 - 3 STEPS



1. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
2. Pd(OAc)2, PPh3, CO, MeCN
3. HCl, Water, DMF

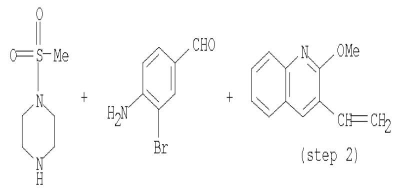
RX(191) OF 350 - 3 STEPS



HCl
100%

NOTE: 1) stereoselective
CON: STEP(1) 4 hours, 100 deg C
STEP(2) 15 hours, 70 deg C, 60 atm

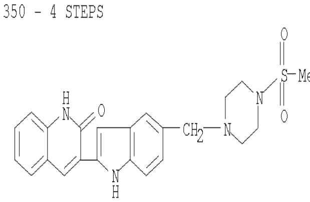
RX(192) OF 350 - 4 STEPS



(step 2)

1.1. Na.(AcO)3BH, CH2Cl2
1.2. NH4Cl, Water
2. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
3. Pd(OAc)2, 1,10-Phenanthroline, CO, DMF
4. HCl, Water, DMF

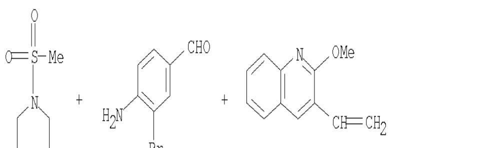
RX(192) OF 350 - 4 STEPS



HCl
100%

NOTE: 2) stereoselective
CON: STEP(1.1) 4 hours, room temperature
STEP(1.2) room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 14 hours, 70 deg C, 15 psi

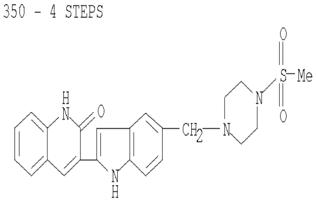
RX(193) OF 350 - 4 STEPS



(step 2)

1.1. Na.(AcO)3BH,
     CH2Cl2
1.2. NH4Cl, Water
2. Tri-o-tolylphosphine,
   Pd(OAc)2, Et3N,
   DMF
3. Pd(OAc)2, PPh3, CO,
   MeCN
4. HCl, Water, DMF

RX(193) OF 350 - 4 STEPS

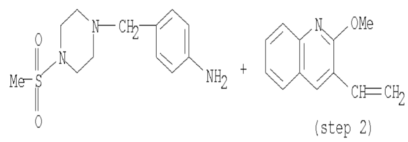


HCl

100%

NOTE: 2) stereoselective
CON: STEP(1.1) 4 hours, room temperature
     STEP(1.2) room temperature
     STEP(2) 4 hours, 100 deg C
     STEP(3) 15 hours, 70 deg C, 60 atm

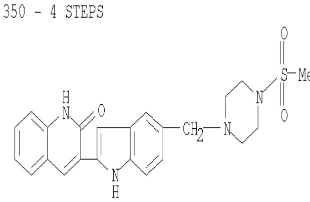
RX(194) OF 350 - 4 STEPS



(step 2)

1. C:98327-87-8,
   R:338746-12-6, KBr,
   Water, AcOH
2. Tri-o-tolylphosphine,
   Pd(OAc)2, Et3N,
   DMF
3. Pd(OAc)2,
   1,10-Phenanthroline,
   CO, DMF
4. HCl, Water, DMF

RX(194) OF 350 - 4 STEPS



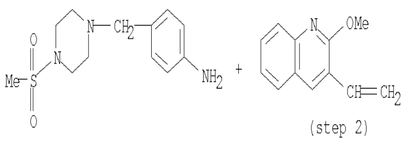
HCl

100%

NOTE: 2) stereoselective
CON: STEP(1) 4 hours, room temperature
     STEP(2) 4 hours, 100 deg C
     STEP(3) 14 hours, 70 deg C, 15 psi

Print selected from 10562215.trn

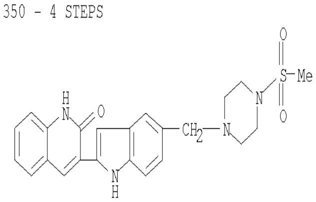
RX(195) OF 350 - 4 STEPS



(step 2)

1. C:98327-87-8, R:338746-12-6, KBr, Water, AcOH
2. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
3. Pd(OAc)2, PPh3, CO, MeCN
4. HCl, Water, DMF

RX(195) OF 350 - 4 STEPS



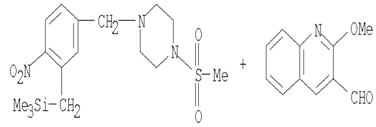
HCl

100%

NOTE: 2) stereoselective
CON: STEP(1) 4 hours, room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 15 hours, 70 deg C, 60 atm

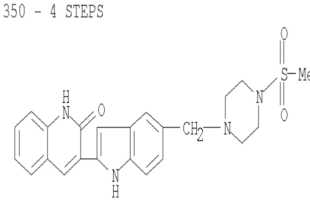
Print selected from 10562215.trn

RX(196) OF 350 - 4 STEPS



1. Bu4N.F, S:108-21-4
2.1. (CF3CO)2O, S:108-21-4
2.2. DBU
3. Pd(OAc)2, 1,10-Phenanthroline, CO, DMF
4. HCl, Water, DMF

RX(196) OF 350 - 4 STEPS

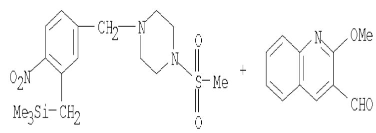


HCl

100%

NOTE: 1) key intermediate, 2) stereoselective
CON: STEP(1.1) room temperature; 30 minutes, room temperature
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 30 minutes, 60 deg C
STEP(3) 14 hours, 70 deg C, 15 psi

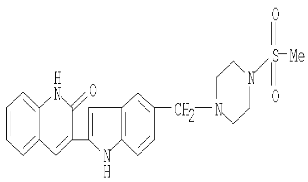
RX(197) OF 350 - 4 STEPS



1. Bu4N.F, S:108-21-4
2.1. (CF3CO)2O, S:108-21-4
2.2. DBU
3. Pd(OAc)2, PPh3, CO, MeCN
4. HCl, Water, DMF

Print selected from 10562215.trn

RX(197) OF 350 - 4 STEPS

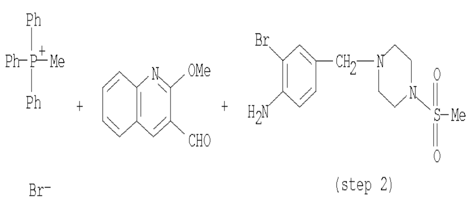


HCl

100%

NOTE: 1) key intermediate, 2) stereoselective
CON: STEP(1.1) room temperature; 30 minutes, room temperature
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 30 minutes, 60 deg C
STEP(3) 15 hours, 70 deg C, 60 atm

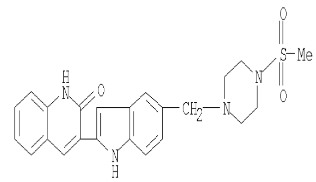
RX(198) OF 350 - 4 STEPS



1.1. BuLi, THF
1.2. THF
2. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
3. Pd(OAc)2, 1,10-Phenanthroline, CO, DMF
4. HCl, Water, DMF

Print selected from 10562215.trn

RX(198) OF 350 - 4 STEPS

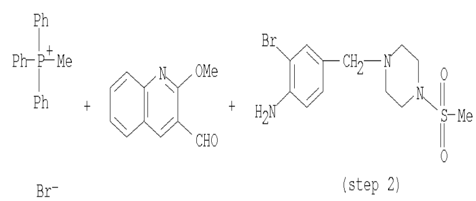


HCl

100%

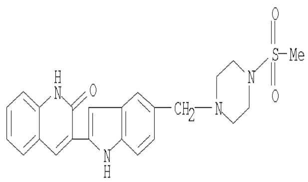
NOTE: 2) stereoselective
CON: STEP(1.1) 30 minutes, room temperature
STEP(1.2) 1 hour, room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 14 hours, 70 deg C, 15 psi

RX(199) OF 350 - 4 STEPS



1.1. BuLi, THF
1.2. THF
2. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
3. Pd(OAc)2, PPh3, CO, MeCN
4. HCl, Water, DMF

RX(199) OF 350 - 4 STEPS

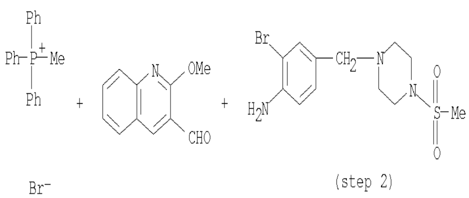


HCl

100%

NOTE: 2) stereoselective
CON: STEP(1.1) 30 minutes, room temperature
STEP(1.2) 1 hour, room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 15 hours, 70 deg C, 60 atm

RX(201) OF 350 - 3 STEPS

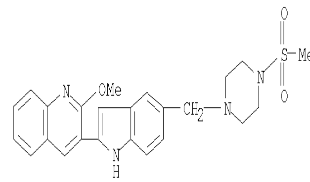


(step 2)

1.1. BuLi, THF
1.2. THF
2. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
3. Pd(OAc)2, 1,10-Phenanthroline, CO, DMF

Print selected from 10562215.trn

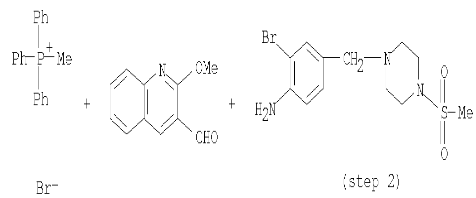
RX(201) OF 350 - 3 STEPS



94%

NOTE: 2) stereoselective
CON: STEP(1.1) 30 minutes, room temperature
STEP(1.2) 1 hour, room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 14 hours, 70 deg C, 15 psi

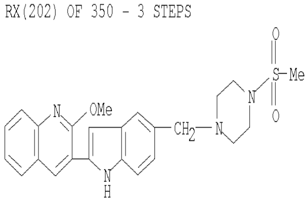
RX(202) OF 350 - 3 STEPS



(step 2)

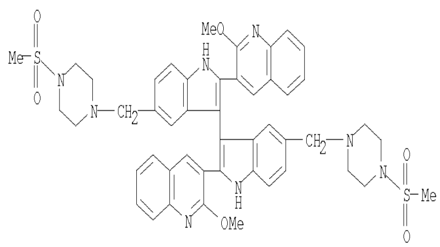
1.1. BuLi, THF
1.2. THF
2. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
3. Pd(OAc)2, PPh3, CO, MeCN

RX(202) OF 350 - 3 STEPS



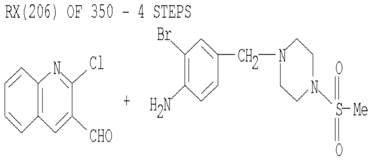
+

95%



NOTE: 2) stereoselective
CON: STEP(1.1) 30 minutes, room temperature
STEP(1.2) 1 hour, room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 15 hours, 70 deg C, 60 atm

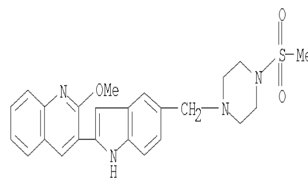
RX(206) OF 350 - 4 STEPS



(step 3)

1. MeOH, KOH
2.1. Ph3PMe.Br, BuLi, THF
2.2. THF
3. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
4. Pd(OAc)2, 1,10-Phenanthroline, CO, DMF

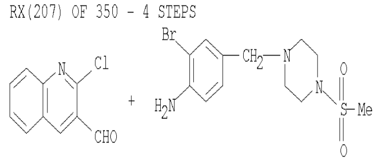
RX(206) OF 350 - 4 STEPS



94%

NOTE: 3) stereoselective
CON: STEP(1) 2.5 hours, reflux
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 1 hour, room temperature
STEP(3) 4 hours, 100 deg C
STEP(4) 14 hours, 70 deg C, 15 psi

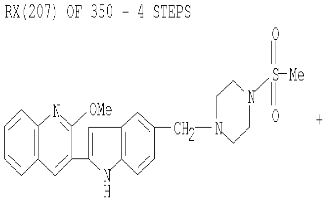
RX(207) OF 350 - 4 STEPS



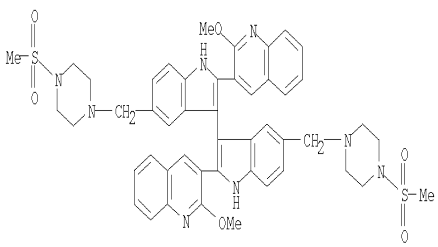
(step 3)

1. MeOH, KOH
2.1. Ph3PMe.Br, BuLi, THF
2.2. THF
3. Tri-o-tolylphosphine, Pd(OAc)2, Et3N, DMF
4. Pd(OAc)2, PPh3, CO, MeCN

RX(207) OF 350 - 4 STEPS



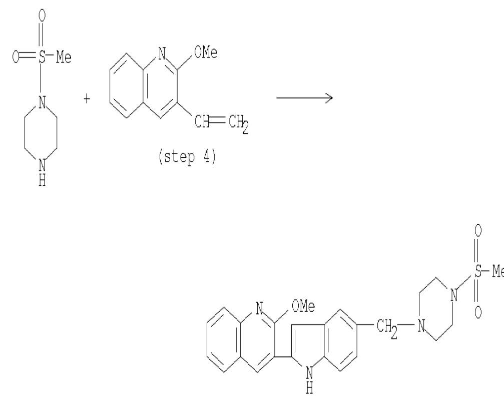
95%



NOTE: 3) stereoselective
CON: STEP(1) 2.5 hours, reflux
STEP(2.1) 30 minutes, room temperature
STEP(2.2) 1 hour, room temperature
STEP(3) 4 hours, 100 deg C
STEP(4) 15 hours, 70 deg C, 60 atm

Print selected from 10562215.trn

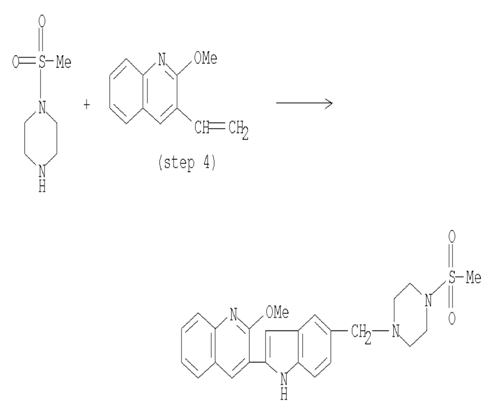
RX(214) OF 350 - 5 STEPS



94%

NOTE: 4) stereoselective
CON: STEP(1.1) 0 deg C; 2 hours, room temperature
STEP(2) 4 hours, room temperature
STEP(3) 4 hours, room temperature
STEP(4) 4 hours, 100 deg C
STEP(5) 14 hours, 70 deg C, 15 psi

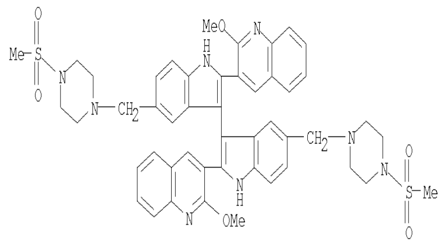
RX(215) OF 350 - 5 STEPS



95%

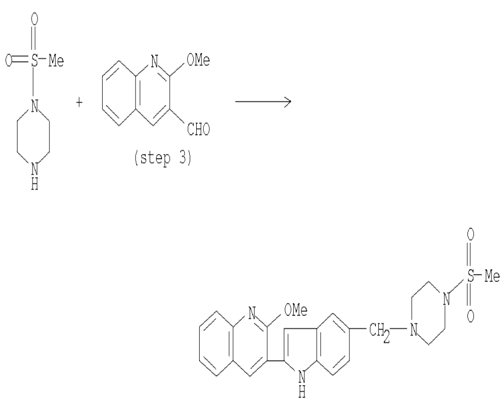
Print selected from 10562215.trn

RX(215) OF 350 - 5 STEPS



NOTE: 4) stereoselective
CON: STEP(1.1) 0 deg C; 2 hours, room temperature
STEP(2) 4 hours, room temperature
STEP(3) 4 hours, room temperature
STEP(4) 4 hours, 100 deg C
STEP(5) 15 hours, 70 deg C, 60 atm

RX(220) OF 350 - 5 STEPS

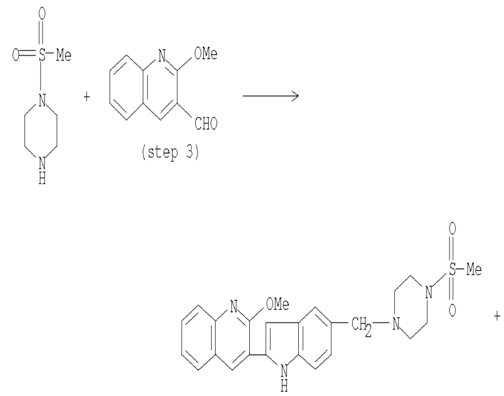


94%

NOTE: 3) key intermediate, 4) stereoselective
CON: STEP(1.1) 0 deg C; 2 hours, room temperature
STEP(2.1) -20 deg C; <-5 deg C; 30 minutes, -20 deg C
STEP(2.2) 3 hours, room temperature
STEP(3.1) room temperature; 30 minutes, room temperature
STEP(4.1) 30 minutes, room temperature
STEP(4.2) 30 minutes, 60 deg C
STEP(5) 14 hours, 70 deg C, 15 psi

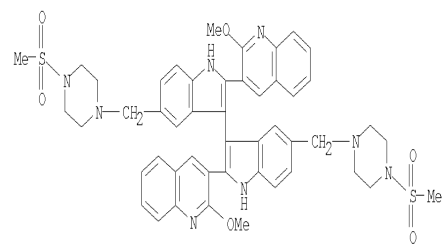
Print selected from 10562215.trn

RX(221) OF 350 - 5 STEPS



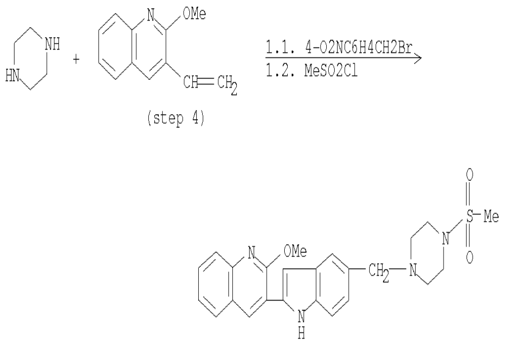
95%

RX(221) OF 350 - 5 STEPS



NOTE: 3) key intermediate, 4) stereoselective
CON: STEP(1.1) 0 deg C; 2 hours, room temperature
STEP(2.1) -20 deg C; <-5 deg C; 30 minutes, -20 deg C
STEP(2.2) 3 hours, room temperature
STEP(3.1) room temperature; 30 minutes, room temperature
STEP(4.1) 30 minutes, room temperature
STEP(4.2) 30 minutes, 60 deg C
STEP(5) 15 hours, 70 deg C, 60 atm

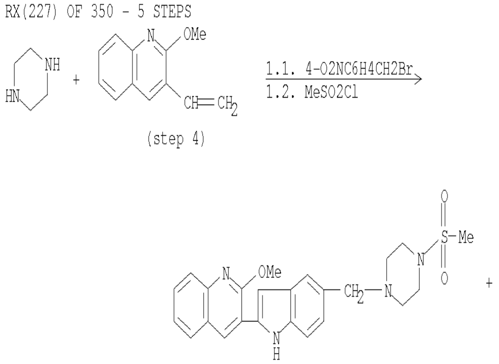
RX(226) OF 350 - 5 STEPS



94%

NOTE: 4) stereoselective
CON: STEP(1.1) 20 minutes, 0 deg C; 30 minutes, room temperature
STEP(1.2) 30 minutes, room temperature
STEP(2) 4 hours, room temperature
STEP(3) 4 hours, room temperature
STEP(4) 4 hours, 100 deg C
STEP(5) 14 hours, 70 deg C, 15 psi

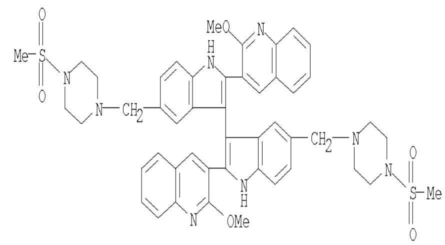
RX(227) OF 350 - 5 STEPS



95%

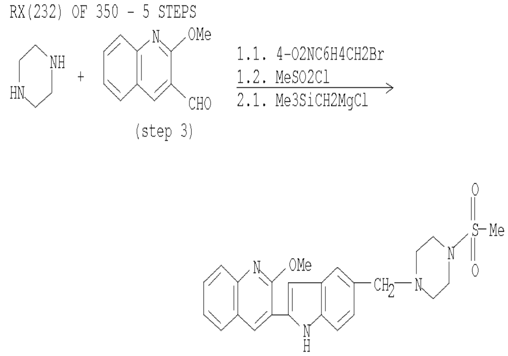
Print selected from 10562215.trn

RX(227) OF 350 - 5 STEPS



NOTE: 4) stereoselective
CON: STEP(1.1) 20 minutes, 0 deg C; 30 minutes, room temperature
STEP(1.2) 30 minutes, room temperature
STEP(2) 4 hours, room temperature
STEP(3) 4 hours, room temperature
STEP(4) 4 hours, 100 deg C
STEP(5) 15 hours, 70 deg C, 60 atm

RX(232) OF 350 - 5 STEPS

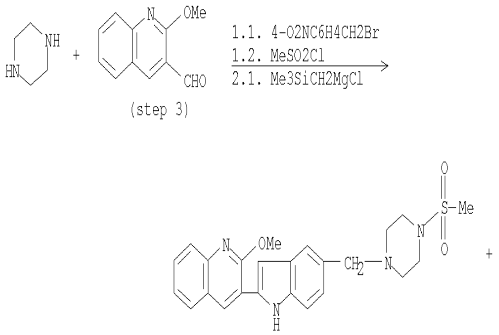


94%

NOTE: 3) key intermediate, 4) stereoselective
CON: STEP(1.1) 20 minutes, 0 deg C; 30 minutes, room temperature
STEP(1.2) 30 minutes, room temperature
STEP(2.1) -20 deg C; <-5 deg C; 30 minutes, -20 deg C
STEP(2.2) 3 hours, room temperature
STEP(3.1) room temperature; 30 minutes, room temperature
STEP(4.1) 30 minutes, room temperature
STEP(4.2) 30 minutes, 60 deg C
STEP(5) 14 hours, 70 deg C, 15 psi

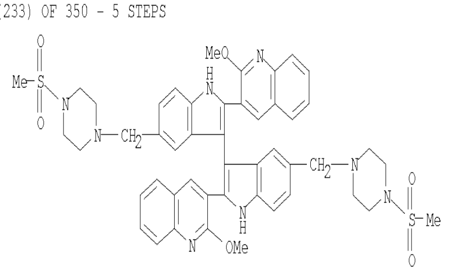
Print selected from 10562215.trn

RX(233) OF 350 - 5 STEPS



95%

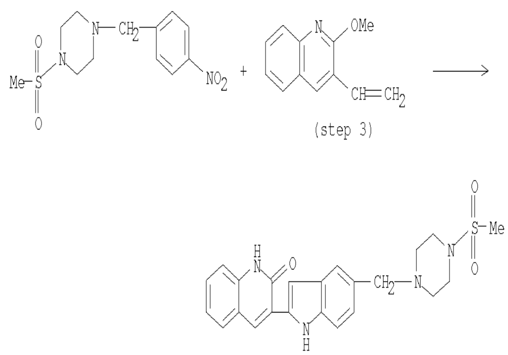
RX(233) OF 350 - 5 STEPS



NOTE: 3) key intermediate, 4) stereoselective
CON: STEP(1.1) 20 minutes, 0 deg C; 30 minutes, room temperature
STEP(1.2) 30 minutes, room temperature
STEP(2.1) -20 deg C; <-5 deg C; 30 minutes, -20 deg C
STEP(2.2) 3 hours, room temperature
STEP(3.1) room temperature; 30 minutes, room temperature
STEP(4.1) 30 minutes, room temperature
STEP(4.2) 30 minutes, 60 deg C
STEP(5) 15 hours, 70 deg C, 60 atm

Print selected from 10562215.trn

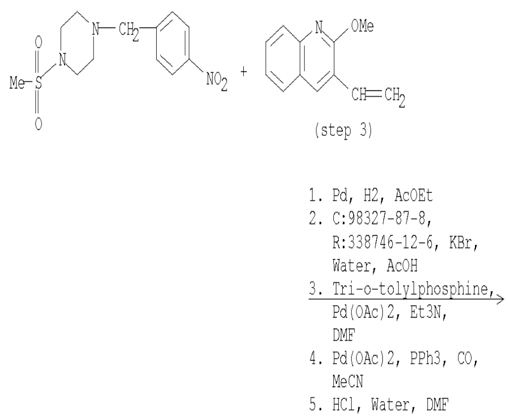
RX(234) OF 350 - 5 STEPS



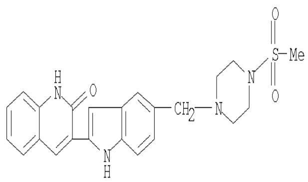
HCl
100%

NOTE: 3) stereoselective
CON: STEP(1) 4 hours, room temperature
STEP(2) 4 hours, room temperature
STEP(3) 4 hours, 100 deg C
STEP(4) 14 hours, 70 deg C, 15 psi

RX(235) OF 350 - 5 STEPS



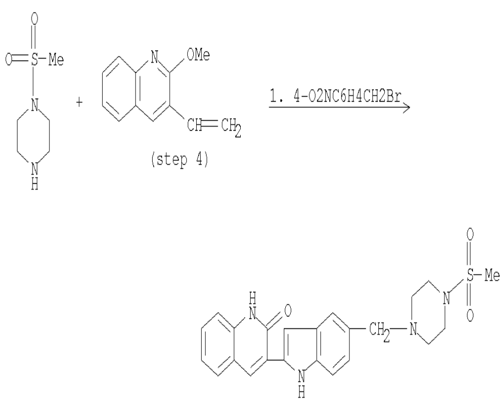
RX(235) OF 350 - 5 STEPS



HCl
100%

NOTE: 3) stereoselective
CON: STEP(1) 4 hours, room temperature
STEP(2) 4 hours, room temperature
STEP(3) 4 hours, 100 deg C
STEP(4) 15 hours, 70 deg C, 60 atm

RX(237) OF 350 - 6 STEPS

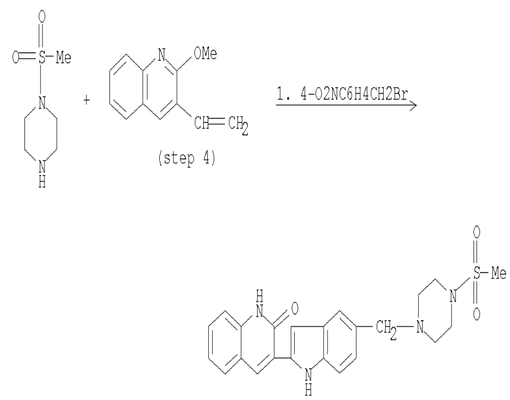


HCl
100%

NOTE: 4) stereoselective
CON: STEP(1.1) 0 deg C; 2 hours, room temperature
STEP(2) 4 hours, room temperature
STEP(3) 4 hours, room temperature
STEP(4) 4 hours, 100 deg C
STEP(5) 14 hours, 70 deg C, 15 psi

Print selected from 10562215.trn

RX(238) OF 350 - 6 STEPS

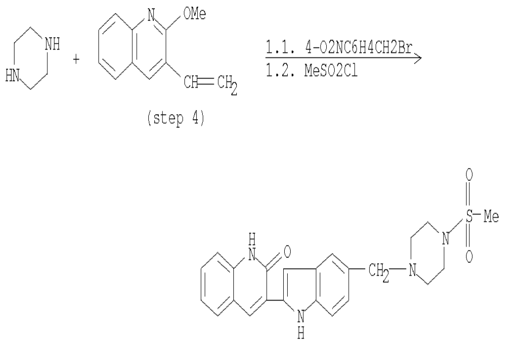


HCl
100%

NOTE: 4) stereoselective
CON: STEP(1.1) 0 deg C; 2 hours, room temperature
STEP(2) 4 hours, room temperature
STEP(3) 4 hours, room temperature
STEP(4) 4 hours, 100 deg C
STEP(5) 15 hours, 70 deg C, 60 atm

Print selected from 10562215.trn

RX(240) OF 350 - 6 STEPS

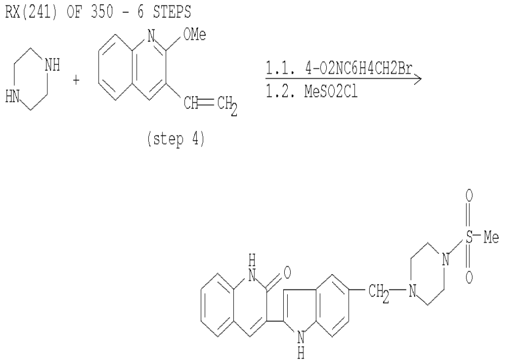


HCl

100%

NOTE: 4) stereoselective
CON: STEP(1.1) 20 minutes, 0 deg C; 30 minutes, room temperature
STEP(1.2) 30 minutes, room temperature
STEP(2) 4 hours, room temperature
STEP(3) 4 hours, room temperature
STEP(4) 4 hours, 100 deg C
STEP(5) 14 hours, 70 deg C, 15 psi

RX(241) OF 350 - 6 STEPS



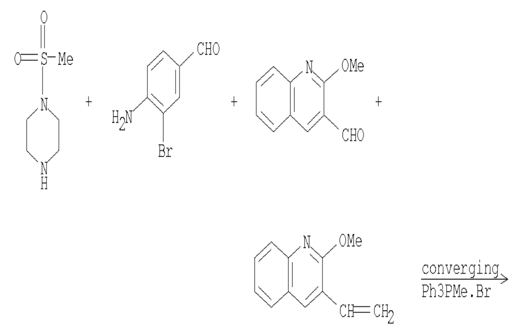
HCl

100%

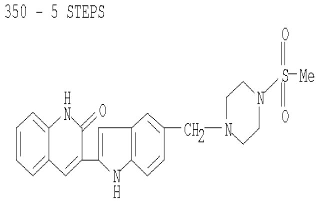
Print selected from 10562215.trn

NOTE: 4) stereoselective
CON: STEP(1.1) 20 minutes, 0 deg C; 30 minutes, room temperature
STEP(1.2) 30 minutes, room temperature
STEP(2) 4 hours, room temperature
STEP(3) 4 hours, room temperature
STEP(4) 4 hours, 100 deg C
STEP(5) 15 hours, 70 deg C, 60 atm

RX(244) OF 350 - 5 STEPS



RX(244) OF 350 - 5 STEPS

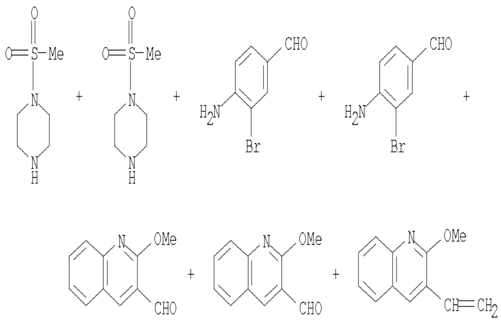


HCl

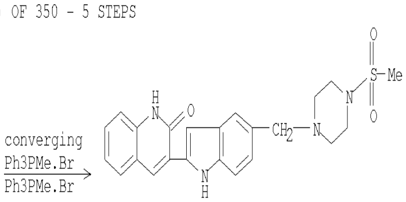
100%

NOTE: stereoselective
CON: STEP(1.1) 4 hours, room temperature
STEP(1.2) room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 14 hours, 70 deg C, 15 psi
STEP(5.1) 30 minutes, room temperature
STEP(5.2) 1 hour, room temperature

RX(245) OF 350 - 5 STEPS



RX(245) OF 350 - 5 STEPS



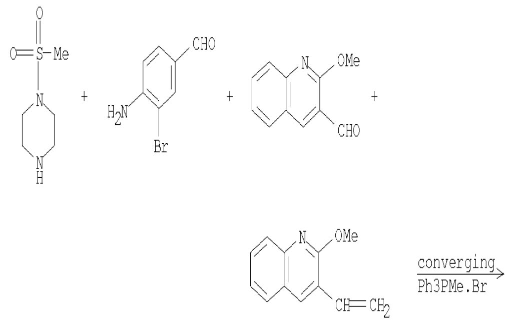
HCl

100%

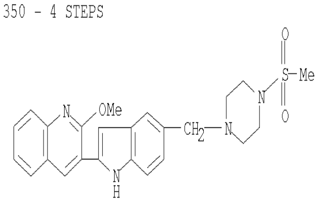
NOTE: stereoselective
CON: STEP(1.1) 4 hours, room temperature
STEP(1.2) room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 15 hours, 70 deg C, 60 atm
STEP(5.1) 30 minutes, room temperature
STEP(5.2) 1 hour, room temperature

Print selected from 10562215.trn

RX(247) OF 350 - 4 STEPS



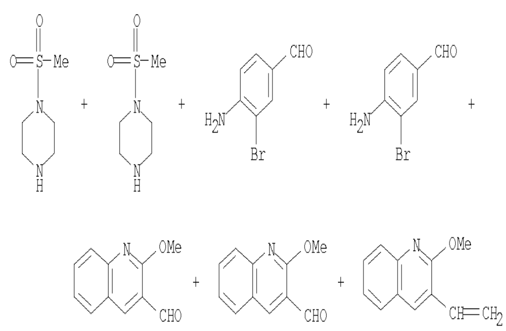
RX(247) OF 350 - 4 STEPS



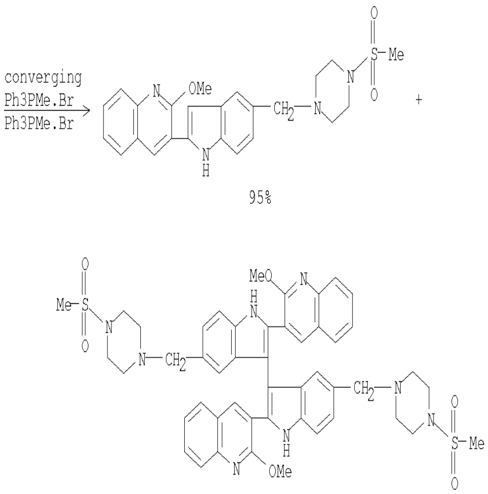
94%

NOTE: stereoselective
CON: STEP(1.1) 4 hours, room temperature
STEP(1.2) room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 14 hours, 70 deg C, 15 psi
STEP(4.1) 30 minutes, room temperature
STEP(4.2) 1 hour, room temperature

RX(248) OF 350 - 4 STEPS

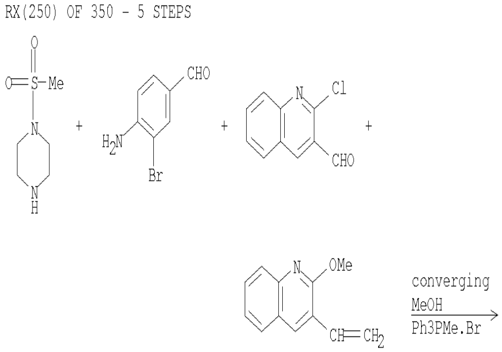


RX(248) OF 350 - 4 STEPS



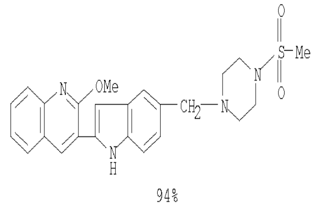
NOTE: stereoselective
CON: STEP(1.1) 4 hours, room temperature
STEP(1.2) room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 15 hours, 70 deg C, 60 atm
STEP(4.1) 30 minutes, room temperature
STEP(4.2) 1 hour, room temperature

RX(250) OF 350 - 5 STEPS



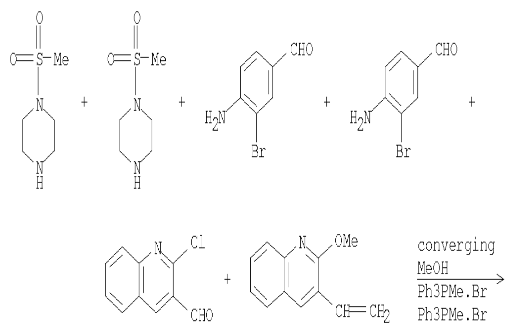
Print selected from 10562215.trn

RX(250) OF 350 - 5 STEPS



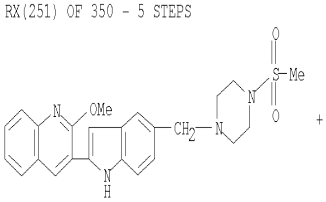
NOTE: stereoselective
CON: STEP(1.1) 4 hours, room temperature
STEP(1.2) room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 14 hours, 70 deg C, 15 psi
STEP(4) 2.5 hours, reflux
STEP(5.1) 30 minutes, room temperature
STEP(5.2) 1 hour, room temperature

RX(251) OF 350 - 5 STEPS

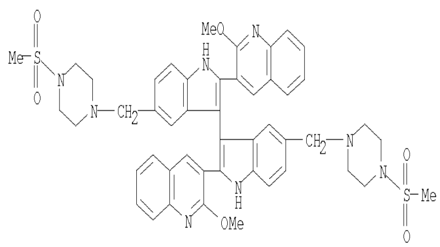


Print selected from 10562215.trn

RX(251) OF 350 - 5 STEPS

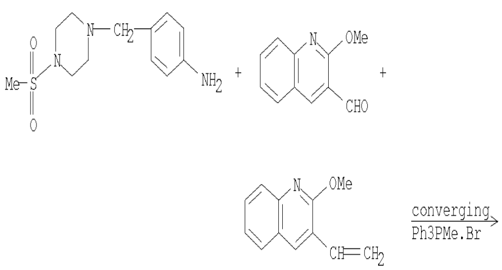


95%



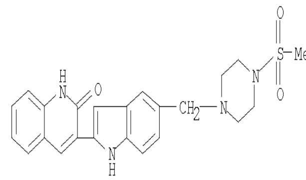
NOTE: stereoselective
CON: STEP(1.1) 4 hours, room temperature
STEP(1.2) room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 15 hours, 70 deg C, 60 atm
STEP(4) 2.5 hours, reflux
STEP(5.1) 30 minutes, room temperature
STEP(5.2) 1 hour, room temperature

RX(253) OF 350 - 5 STEPS



Print selected from 10562215.trn

RX(253) OF 350 - 5 STEPS

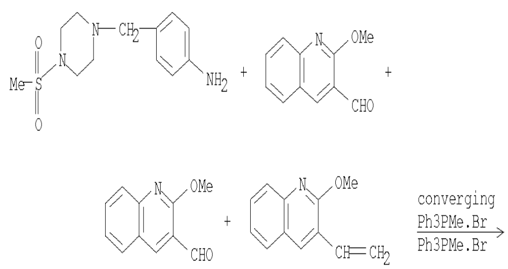


HCl

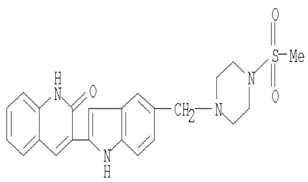
100%

NOTE: stereoselective
CON: STEP(1) 4 hours, room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 14 hours, 70 deg C, 15 psi
STEP(5.1) 30 minutes, room temperature
STEP(5.2) 1 hour, room temperature

RX(254) OF 350 - 5 STEPS



RX(254) OF 350 - 5 STEPS

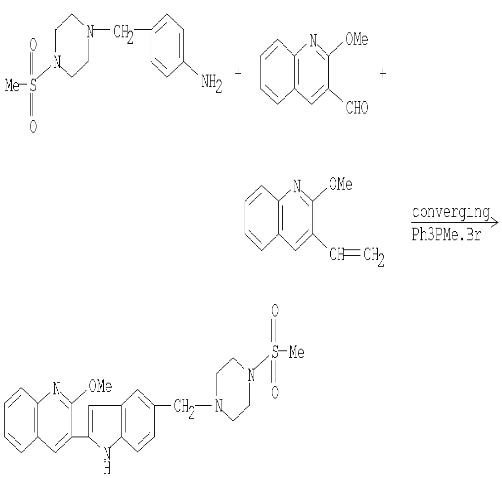


HCl

100%

NOTE: stereoselective
CON: STEP(1) 4 hours, room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 15 hours, 70 deg C, 60 atm
STEP(5.1) 30 minutes, room temperature
STEP(5.2) 1 hour, room temperature

RX(256) OF 350 - 4 STEPS



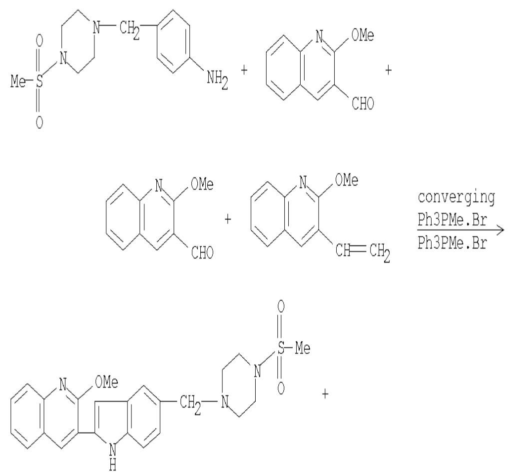
94%

<------User Break------>

NOTE: stereoselective
CON: STEP(1) 4 hours, room temperature
STEP(2) 4 hours, 100 deg C
STEP(3) 14 hours, 70 deg C, 15 psi
STEP(4.1) 30 minutes, room temperature
STEP(4.2) 1 hour, room temperature

Print selected from 10562215.trn

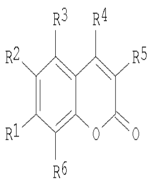
RX(257) OF 350 - 4 STEPS



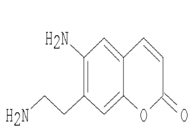
95%

=> d cbib abs fcrd 1-
YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/(N):y

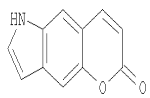
L8 ANSWER 1 OF 2 CASREACT COPYRIGHT 2009 ACS on STN
144:292572 Diaminocoumarins as fluorogenic substrates for monoamine oxidases, and their preparation, pharmaceutical compositions, photophysical properties, and a method for detecting active monoamine oxidases and their inhibitors for treatment of nervous system disorders. Chen, Gong; Yee, Dominic J.; Gubernator, Niko; Sames, Dalibor (The Trustees of Columbia University in the City of New York, USA). PCT Int. Appl. WO 2006026368 A2 20060309, 278 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IS, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2005-US30276 20050825. PRIORITY: US 2004-604538P 20040825.
GI



I



II

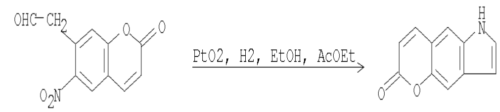


III

AB The invention relates to compds. of formula I, which are useful for detecting the activity of monoamine oxidases (MAO), compds. useful for competitively inhibiting monoamine oxidases, for determining inhibitors of monoamine oxidases and compds. useful for treating monoamine oxidase-related nervous system pathologies, as well as pharmaceutical compns. and methods of manufacture thereof. Compds. of formula I wherein R1 is H, alkyl, alkenyl, alkynyl, (un)substituted (hetero)aryl, cycloalkyl, NH2 and derivs., alkyl-CO2H, alkyl-OH, alkyl-NH2, halo, CX3, or indole; R2-R6 are independently H, OH, alkyl, alkenyl, alkynyl, (un)substituted (hetero)aryl, cycloalkyl, NH2 and derivs., alkyl-CO2H, alkyl-OH, alkyl-NH2, O-alkyl, O-alkenyl, O-alkynyl, O-aryl, O-cycloalkyl, CX3, halo, or indole; R1R2 and R1R6 may independently form an unsubstituted pyrrole; R1R2R6 may form an octahydroquinazolizine; R2R3 may form a pyrrole; X is halo; or pharmaceutically acceptable salts, or stereoisomers thereof are claimed in this invention. The process for preparing these fluorogenic substrates, and a method for identifying a test compound as a substrate of MAO are also claimed. Example compound II was prepared by nitration of 7-methylcoumarin, and the resulting 7-methyl-6-nitrocoumarin underwent condensation with DMF di-Me acetal to give the corresponding coumarin-enamine, which was hydrolyzed to give 7-(2-oxoethyl)-6-nitrocoumarin, which underwent reductive amination with dibenzosuberylamine; the resulting 7-(dibenzosuberylaminoethyl)-6-nitrocoumarin was reduced to the 6-aminocoumarin compound, which was hydrolyzed to give coumarin II. The invention compds. were evaluated for their photophys. properties and their enzymic activity toward MAO-A and MAO-B. Coumarin II showed λmax 352 nm, ε 2000±100 M-1cm-1, Φ 0.0017±0.0001, and λem was not detected. The invention compds. were evaluated for their ability to convert to the corresponding indole in the presence of MAO-A and MAO-B. Enzyme-catalyzed indole formation was realized after 24 h by reading fluorescence emission upon excitation at the absorbance maxima of the resp. indoles. Only diamino-coumarin II showed a significant conversion to its indole III in the presence of MAO-A and MAO-B. The enzyme kinetics for fluorogenic probe II were also determined Compound II showed for MAO-A: Km = 30.9±1.8 μM, Kcat = 0.475 min-1, Kcat/Km = 0.015 min-1 μM-1, Vmax(mitochondria) = 0.0570 nmol min-1 mg-1; and for MAO-B: Km = 510±40 μM, Kcat = 20.62 min-1, Kcat/Km = 0.040 min-1 μM-1, and Vmax(mitochondria) = 1.2 nmol min-1 mg-1. These results indicate that coumarin probe II is a good substrate for monoamine oxidase and could be useful as a fluorescent reporter for monoamine oxidase.

Print selected from 10562215.trn

RX(15) OF 512



83%

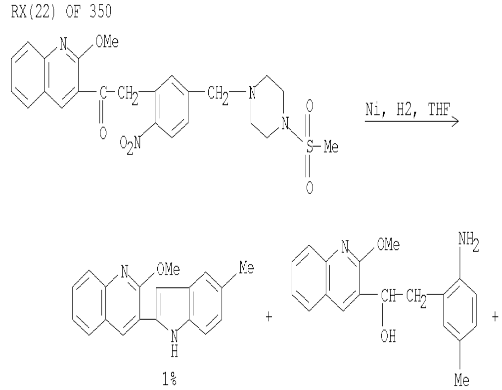
CON: 2 hours, room temperature

L8 ANSWER 2 OF 2 CASREACT COPYRIGHT 2009 ACS on STN
142:411180 Synthesis of 5-Substituted-1H-indol-2-yl-1H-quinolin-2-ones: A Novel Class of KDR Kinase Inhibitors. Kuethe, Jeffrey T.; Wong, Audrey; Qu, Chuanxing; Smitrovich, Jacqueline; Davies, Ian W.; Hughes, David L. (Department of Process Research, Merck & Co., Inc., Rahway, NJ, 07065, USA). Journal of Organic Chemistry, 70(7), 2555-2567 (English) 2005. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

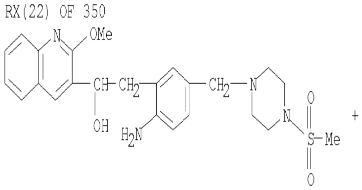
AB A number of approaches for the synthesis of the 1H-indol-2-yl-1H-quinolin-2-one ring system found in the potent and selective KDR kinase inhibitor I are described. The preparation and reaction of trimethylsilylnitrobenzene II with 2-methoxy-3-quinolinecarboxaldehyde afforded alc. III, which was the key intermediate for the preparation of the target compds. Conversion of alc. III to either nitroketone IV or nitrostyrene V set the stage for reductive cyclization. The quinolin-2-one functionality was unmasked in the last step to provide compound I in 56-60% overall yield from readily available starting materials.

RX(22) OF 350



1% 1%

RX(22) OF 350



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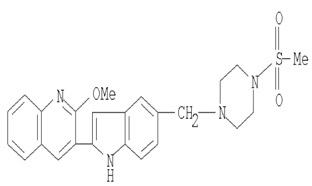

90%

NOTE: Raney Nickel used
CON: 7.5 hours, 65 deg C, 40 psi

=>
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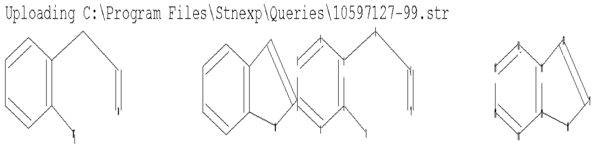
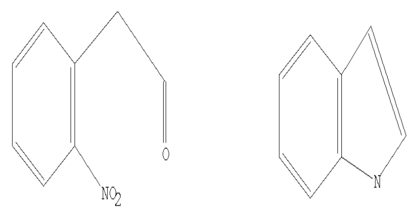


chain nodes :
7 8 9
ring nodes :
1 2 3 4 5 6 11 12 13 14 15 16 17 18 19
ring/chain nodes :
10
chain bonds :
5-8 6-7 8-9 9-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 15-17 16-19
17-18 18-19
exact/norm bonds :
9-10 15-17 16-19 17-18 18-19
exact bonds :
5-8 6-7 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
fragments assigned product role:
containing 11
fragments assigned reactant/reagent role:
containing 1
node mappings:
6:16 6:16

L9   STRUCTURE UPLOADED

=> d l9
L9 HAS NO ANSWERS
L9   STR



Structure attributes must be viewed using STN Express query preparation.

=> s l9
SAMPLE SEARCH INITIATED 11:21:40 FILE 'CASREACT'
SCREENING COMPLETE -   268 REACTIONS TO VERIFY FROM   26 DOCUMENTS

100.0% DONE   268 VERIFIED   76 HIT RXNS   6 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS: 4378 TO   6342
PROJECTED ANSWERS: 6 TO   266

L10   6 SEA SSS SAM L9 (76 REACTIONS)

=> s l9 full
FULL SEARCH INITIATED 11:21:48 FILE 'CASREACT'
SCREENING COMPLETE -   6095 REACTIONS TO VERIFY FROM   502 DOCUMENTS

100.0% DONE   6095 VERIFIED   1697 HIT RXNS (120 INCOMP)   151 DOCS
SEARCH TIME: 00.00.02

L11   151 SEA SSS FUL L9 (1697 REACTIONS)

=> d his

(FILE 'HOME' ENTERED AT 11:15:49 ON 16 MAR 2009)

FILE 'CASREACT' ENTERED AT 11:16:04 ON 16 MAR 2009
L1 STRUCTURE UPLOADED
L2 3 S L1
L3 114 S L1 FULL
L4 0 S L3 AND CARBON MONOXIDE
L5 5849 S CARBON MONOXIDE

FILE 'REGISTRY' ENTERED AT 11:17:25 ON 16 MAR 2009
L6 1 S CARBON MONOXIDE/CN

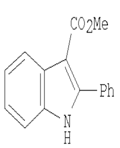
FILE 'CASREACT' ENTERED AT 11:17:52 ON 16 MAR 2009
L7 10878 S 630-08-0
L8 2 S L7 AND L3
L9 STRUCTURE UPLOADED
L10 6 S L9
L11 151 S L9 FULL

=> s l11 and l7
L12 3 L11 AND L7

=> s l12 not l8
L13 1 L12 NOT L8

=> d cbib abs fcrd

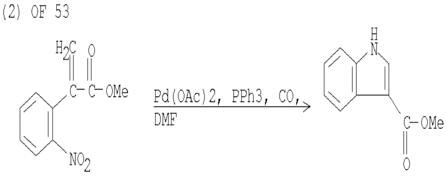
L13 ANSWER 1 OF 1 CASREACT COPYRIGHT 2009 ACS on STN
149:79436 Palladium-catalyzed synthesis of 3-indolecarboxylic acid derivatives. Soderberg, Bjorn C. G.; Banini, Serge R.; Turner, Michael R.; Minter, Aaron R.; Arrington, Amanda K. (C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV, 26506-6045, USA). Synthesis (6), 903-912 (English) 2008. CODEN: SYNTBF. ISSN: 0039-7881. Publisher: Georg Thieme Verlag.
GI



I

AB Indoles having an ester functionality in the 3-position, e.g., I, were prepared from 2-(2-nitrophenyl)propenoic acid derivs. via a palladium-catalyzed reductive N-heteroannulation using carbon monoxide as the ultimate reducing agent. The starting materials were prepared either by a Stille coupling of 2-halo-1-nitrobenzenes with Et 2-(tributylstannyl)-2-propenoate or by vicarious nucleophilic substitution of nitrobenzenes followed by a Knoevenagel-type condensation with an aldehyde. Synthesis of an example of a 3-nitrile- and a 3-sulfone-substituted indole is also described using the same type of methodologies.

RX(2) OF 53



91%

CON: STAGE(1) room temperature; room temperature -> 110 deg C, 6 atm; 72 hours, 110 deg C, 6 atm

=> d his

(FILE 'HOME' ENTERED AT 11:15:49 ON 16 MAR 2009)

FILE 'CASREACT' ENTERED AT 11:16:04 ON 16 MAR 2009
L1 STRUCTURE UPLOADED
L2 3 S L1
L3 114 S L1 FULL
L4 0 S L3 AND CARBON MONOXIDE
L5 5849 S CARBON MONOXIDE

FILE 'REGISTRY' ENTERED AT 11:17:25 ON 16 MAR 2009
L6 1 S CARBON MONOXIDE/CN

FILE 'CASREACT' ENTERED AT 11:17:52 ON 16 MAR 2009
L7 10878 S 630-08-0
L8 2 S L7 AND L3
L9 STRUCTURE UPLOADED
L10 6 S L9
L11 151 S L9 FULL
L12 3 S L11 AND L7
L13 1 S L12 NOT L8

=> s help
Enter the terms you wish to use in your search profile.
ENTER LOGIC EXPRESSION, QUERY NAME, OR (END):end
SEARCH ENDED BY USER

=> help sfields

The searchable fields in the CASREACT File are listed below. If you do not specify a field, your term will be searched in the Basic Index, which contains CAS Registry Numbers (R) for reactants, products, reagents, catalysts, and solvents, and single words from the reaction notes, title, supplementary terms, index terms, and abstracts. Simultaneous left and right truncation (SLART), e.g., S ?TOXIN?, may be used for search terms in the /BI and /NTE search fields in CASREACT.

Reaction Fields

Definition Search Code

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Basic Index	/BI or none
Catalyst	/CAT
Functional Group Formed	/FG.FORM
Functional Group in Product	/FG.PRO
Functional Group in Reactant	/FG.RCT
Functional Group in Reactant, Reagent, or Product	/FG
Functional Group in Reagent	/FG.RGT
Functional Group Reacting	/FG.RXN
Functional Group Yield	/FG.YD
Functional Group Yield Data	/FG.YDT
NonProduct	/NPRO
Nonreacting Functional Group	/FG.NON
Number of Steps	/NS
Product	/PRO
Reactant	/RCT
Reactant or Reagent	/RRT
Reaction Notes	/NTE
Reagent	/RGT
Solvent	/SOL
Yield	/YD
Yield Data	/YDT

General Document Search Fields

Definition	Search Code
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Basic Index	/BI
Abstract	/AB
Accession Number	/AN
Author or Inventor	/AU
CA Section Cross-reference	/SX
Classification Code (CA Section)	/CC
Controlled Term	/CT
Controlled Word	/CW
Corporate Source	/CS
Country of Author	/CYA
Crossover Key	/CK
Document Type	/DT
Entry Date	/ED
Field Availability	/FA
File Segment	/FS
Index Term	/IT
International Standard (Document) Number	/ISN
Issue Number of Publication	/IS
Journal Title	/JT
Language	/LA
Other Source	/OS
Publication Date	/PD
Publication Year	/PY
Publisher	/PB
Publisher Item Identifier	/PUI
Source	/SO
Supplementary Term	/ST
Title	/TI
Uniform Resource Locator	/URL

Print selected from 10562215.trn

Update Date	/UP
Volume and Issue of CA	/VI
Volume Number of Publication	/VL

Patent Search Fields

Definition	Search Code
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Designated States	/DS
International Patent Classification (includes Main and Secondary IPC)	/IC
International Patent Classification, Additional or Supplementary	/ICA
International Patent Classification, Index or Complementary	/ICI
International Patent Classification, Main	/ICM
International Patent Classification, Main Group, Range Searchable	/MGR
International Patent Classification, Secondary	/ICS
International Patent Classification, Subgroup, Range Searchable	/SGR
Inventor Name	/IN
National Patent Classification	/NCL
National Patent Classification, Range Searchable	/NCLR
Patent Application Country	/AC
Patent Application Date	/AD
Patent Application Number	/AP
Patent Application Year	/AY
Patent Assignee	/PA
Patent Country	/PC
Patent Kind Code	/PK
Patent Number	/PN
Priority Application Country	/PRC
Priority Application Date	/PRD
Priority Application Number	/PRN
Priority Application Year	/PRY

You may also use the following super search fields to execute a search in one or more patent fields:

Search Field Name	Super Search Code	Fields Searched
International Patent Classifications	/IPC	/IC,/ICA,/ICI
Patent Application and Priority Number	/APPS	/AP,/PRN
Patent Countries	/PCS	/PC,/DS
Patent Numbers	/PATS	/PN

All fields are text fields except Entry Date (/ED), Functional Group Yield (/FG.YD), International Patent Classification, Main Group, Range Searchable (/MGR), International Patent Classification, Subgroup, Range Searchable (/SGR), Issue Number (/IS), National Patent Classification, Range Searchable (/NCLR), Number of Steps (/NS), Patent Application Date (/AD), Patent Application Year (/AY), Priority Application Date (/PRD), Priority Application Year (/PRY),

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 Publication Date (/PD), Publication Year (/PY), Update Date (/UP),
 Volume (/VL) and Yield (/YD), which are numeric and may be searched
 with numeric operators or ranges, e.g., ED>19971230 or 1/NS.

 Search and display fields generally have the same field codes.  To
 see a list of display fields, enter HELP DFIELDS at an arrow prompt
 (=>).


=> d hia
'HIA' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number.  SCAN
             must be entered on the same line as DISPLAY, e.g.,
             D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for
             all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first
             hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
             CA reference information (SO, PY).  (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction
             Summary for all hit reactions and fields containing
             hit terms
OCC -------- All hit fields and the number of occurrences of the
             hit terms in each field.  Includes total number of
             HIT, PATH, SPATH reactions. Labels reactions that have
             incomplete verifications.
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PATH ------- Reaction Map and Reaction Diagram for the "long
             path".  Displays all hit reactions, except those
             whose steps are totally included within another hit
             reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summaries (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
             path".  Displays all single step reactions which
             contain a hit substance.  Also displays those
             multistep reactions that have a hit substance in both
             the first and last steps of the reaction, except for
             those hit reactions whose steps are totally included
             within another hit reaction which is displayed

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS
at an arrow prompt (=>).  Examples of combinations include: D TI;
D BIB RX; D TI, AU, FCRD.  The information is displayed in the same order
as the specification.  All of the formats, except CRD, CRDREF, FHIT, PATH,
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may
be used with the DISPLAY command to display the record for a specified
Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):d his
'D' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
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OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
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             must be entered on the same line as DISPLAY, e.g.,
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SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for
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STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
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             hit reaction
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FSPATH ----- SPATH, plus Reaction Summary for the "short path"
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             Summary for all hit reactions and fields containing
             hit terms
OCC -------- All hit fields and the number of occurrences of the
             hit terms in each field.  Includes total number of
             HIT, PATH, SPATH reactions. Labels reactions that have
             incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long
             path".  Displays all hit reactions, except those
             whose steps are totally included within another hit
             reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
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             path".  Displays all single step reactions which
             contain a hit substance.  Also displays those
             multistep reactions that have a hit substance in both
             the first and last steps of the reaction, except for
             those hit reactions whose steps are totally included
             within another hit reaction which is displayed

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS
at an arrow prompt (=>).  Examples of combinations include: D TI;
D BIB RX; D TI, AU, FCRD.  The information is displayed in the same order
as the specification.  All of the formats, except CRD, CRDREF, FHIT, PATH,
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may
be used with the DISPLAY command to display the record for a specified
Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):end

=> d his

     (FILE 'HOME' ENTERED AT 11:15:49 ON 16 MAR 2009)

     FILE 'CASREACT' ENTERED AT 11:16:04 ON 16 MAR 2009
L1              STRUCTURE UPLOADED
L2            3 S L1
L3          114 S L1 FULL
L4            0 S L3 AND CARBON MONOXIDE
L5         5849 S CARBON MONOXIDE

     FILE 'REGISTRY' ENTERED AT 11:17:25 ON 16 MAR 2009
L6            1 S CARBON MONOXIDE/CN

     FILE 'CASREACT' ENTERED AT 11:17:52 ON 16 MAR 2009
L7        10878 S 630-08-0
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L8            2 S L7 AND L3
L9              STRUCTURE UPLOADED
L10           6 S L9
L11         151 S L9 FULL
L12           3 S L11 AND L7
L13           1 S L12 NOT L8

=> s l11 and iron
         15437 IRON
            12 IRONS
         15437 IRON
                 (IRON OR IRONS)
L14          3 L11 AND IRON

=> s l11 and carbonyl
         35779 CARBONYL
          1939 CARBONYLS
         36380 CARBONYL
                 (CARBONYL OR CARBONYLS)
L15          3 L11 AND CARBONYL

=> s l11 and complex
        100247 COMPLEX
         80122 COMPLEXES
        117248 COMPLEX
                 (COMPLEX OR COMPLEXES)
L16          2 L11 AND COMPLEX

=> s l13-l16
L17          9 (L13 OR L14 OR L15 OR L16)

=> s l14-l16
L18          8 (L14 OR L15 OR L16)

=> s l18 not l12
L19          8 L18 NOT L12

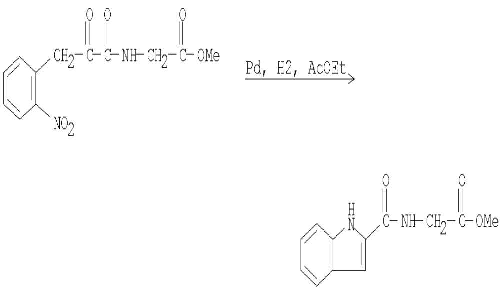
=> s l18 not l8
L20          8 L18 NOT L8

=> d cbib abs fcrd


L20  ANSWER 1 OF 8  CASREACT  COPYRIGHT 2009 ACS on STN
148:449603  Atom-efficient synthesis of 2,6-diazacyclophane compounds through
     alcoholysis/reduction of 3-nitroarylmethylene-2,5-piperazinediones.
     Gonzalez, Juan Francisco; de la Cuesta, Elena; Avendano, Carmen
     (Departamento de Quimica Organica y Farmaceutica, Facultad de Farmacia,
     Universidad Complutense, Madrid, 28040, Spain).  Tetrahedron, 64(12),
     2762-2771 (English) 2008.  CODEN: TETRAB.  ISSN: 0040-4020.  Publisher:
     Elsevier Ltd..
AB   A one-pot ring-opening/alcoholysis/hydrolysis process with
     3-[(nitroaryl)methylene]-2,5-piperazinediones yielded
     N-[3-(nitroaryl)pyruvoyl] amino esters, which gave the corresponding
     amines by reduction of the nitro group.  In the case of 2-nitroaryl compds.,
     an intramol. reductive amination afforded N-(indole-2-carbonyl)
     amino esters, while the intermol. reductive amination of 3- and
     4-nitroaryl derivs. allowed the synthesis of 2,6-diazacyclophanes.  The
     amino compds. may be coupled with amino acids to yield peptide-like
```

derivs.

RX(22) OF 77



92%

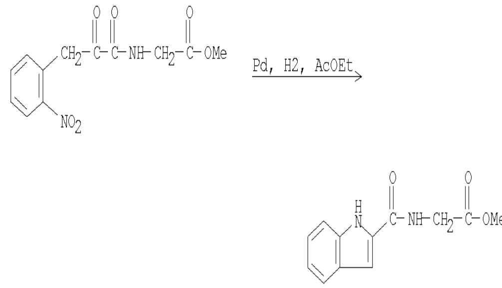
CON: 5 hours, room temperature

=> d cbib abs fcrd 1-
YOU HAVE REQUESTED DATA FROM 8 ANSWERS - CONTINUE? Y/(N):y

L20 ANSWER 1 OF 8 CASREACT COPYRIGHT 2009 ACS on STN
148:449603 Atom-efficient synthesis of 2,6-diazacyclophane compounds through alcoholysis/reduction of 3-nitroarylmethylene-2,5-piperazinediones. Gonzalez, Juan Francisco; de la Cuesta, Elena; Avendano, Carmen (Departamento de Quimica Organica y Farmaceutica, Facultad de Farmacia, Universidad Complutense, Madrid, 28040, Spain). Tetrahedron, 64(12), 2762-2771 (English) 2008. CODEN: TETRAB. ISSN: 0040-4020. Publisher: Elsevier Ltd..

AB A one-pot ring-opening/alcoholysis/hydrolysis process with 3-[(nitroaryl)methylene]-2,5-piperazinediones yielded N-[3-(nitroaryl)pyruvoyl] amino esters, which gave the corresponding amines by reduction of the nitro group. In the case of 2-nitroaryl compds., an intramol. reductive amination afforded N-(indole-2-carbonyl) amino esters, while the intermol. reductive amination of 3- and 4-nitroaryl derivs. allowed the synthesis of 2,6-diazacyclophanes. The amino compds. may be coupled with amino acids to yield peptide-like derivs.

RX(22) OF 77



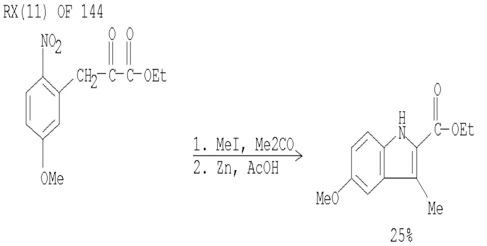
92%

CON: 5 hours, room temperature

L20 ANSWER 2 OF 8 CASREACT COPYRIGHT 2009 ACS on STN
148:23738 Chemistry of Pyrrolo[1,2-a]indole- and Pyrido[1,2-a]indole-Based Quinone Methides. Mechanistic Explanations for Differences in Cytostatic/Cytotoxic Properties. Khdour, Omar; Skibo, Edward B. (Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ, 85287-1604, USA). Journal of Organic Chemistry, 72(23), 8636-8647 (English) 2007. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

AB In the present study the authors investigate pyrido[1,2-a]indole- and pyrrolo[1,2-a]indole-based quinones capable of forming quinone methide and vinyl quinone species upon reduction and leaving group elimination. The goals were to determine the influence of the 6-membered pyrido and the 5-membered pyrrolo fused rings on quinone methide and vinyl quinone formation and fate as well as on cytostatic and cytotoxic activity. The authors used the technique of Spectral Global Fitting to study the fleeting quinone methide intermediate directly. Conclusions regarding quinone methide reactivity are that carbonyl O-protonation is required for nucleophile trapping and that the pKa value of this protonated species is near neutrality. The abnormally high protonated carbonyl pKa values are due to the formation of an aromatic carbocation species upon protonation. The fused pyrido ring promotes quinone methide and vinyl quinone formation but slows nucleophile trapping compared to the fused pyrrolo ring. These findings are explained by the presence of axial hydrogen atoms in the fused pyrido ring resulting in more steric congestion compared to the relatively flat fused pyrrolo ring. Consequently, pyrrolo[1,2-a]indole-based quinones exhibit more cytostatic activity than the pyrido[1,2-a]indole analogs due to their greater nucleophile trapping capability.

RX(11) OF 144



x K

(step 1)

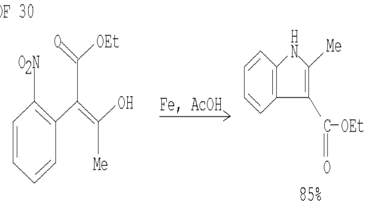
CON: STAGE(1) room temperature; 4 hours, room temperature
STAGE(2) 3 hours, 40 - 45 deg C

L20 ANSWER 3 OF 8 CASREACT COPYRIGHT 2009 ACS on STN

138:204905 2-Alkylindole-3-carboxylate esters by a tandem reduction-addition-elimination reaction. Bunce, Richard A.; Randall, Marty H.; Applegate, Kirby G. (Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078-3071, USA). Organic Preparations and Procedures International, 34(5), 483-489 (English) 2002. CODEN: OPPIAK. ISSN: 0030-4948. Publisher: Organic Preparations and Procedures, Inc..

AB 2-Alkylindole-3-carboxylate esters were prepared by nucleophilic substitution of 1-fluoro-2-nitrobenzene with β-keto ester anions formed from RCOCH2CO2Et (R = alkyl, 3-butenyl, CH2CH2Ph cyclohexyl, Ph, 2-ClC6H4), to give (Z)-2-O2NC6H4C(CO2Et):CR(OH), followed by tandem reduction-addition-elimination using iron powder in glacial acetic acid.

RX(11) OF 30

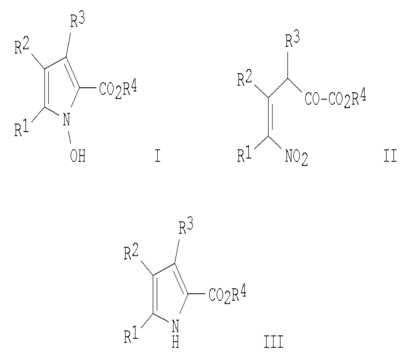


NOTE: Michael addn.
CON: STAGE(1) 115 deg C; 115 deg C -> room temperature

L20 ANSWER 4 OF 8 CASREACT COPYRIGHT 2009 ACS on STN

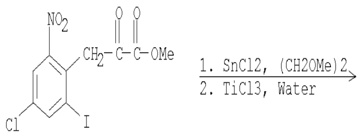
133:266728 Preparation of N-hydroxypyrrole-2-carboxylic acids and pyrrole-2-carboxylic acids. Katayama, Seiji; Ae, Nobuyuki; Nagata, Tatsu (Sumitomo Pharmaceuticals Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2000273084 A 20001003, 13 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1999-77212 19990323.

GI

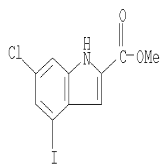


AB N-hydroxypyrrole-2-carboxylic acids I [R1-R3 = H, (un)substituted alkyl, (un)substituted aryl, (un)substituted heteroaryl; R1 and R2 may be bonded together to form a condensed aromatic ring; R2 and R3 may be bonded together to form a condensed cycloalkane or heterocycloalkane ring; R4 = (un)substituted alkyl], useful as intermediates for drugs and agrochems., are prepared by treating nitro keto esters II (R1-R4 = same as above) with reducing agents. Pyrrole-2-carboxylic acids III (R1-R4 = same as above), also useful as intermediates for drugs and agrochems., are prepared by treating II with reducing agents and reacting the resulting I with other reducing agents. A dimethoxyethane solution of Me (2-iodo-4-chloro-6-nitrophenyl)pyruvate [preparation from 4-chloro-2-nitrotoluene (IV) with 2 steps] was gradually added to a H2O/dimethoxyethane solution of SnCl2 at room temperature and the reaction mixture was further stirred for 1 h. An aqueous TiCl3 solution was gradually added to the above reaction mixture at 0° and the mixture was stirred for 1 h to give 51% (based on IV) Me 4-iodo-6-chloroindole-2-carboxylate. Preparation of 3-(S)-3-[2-(1-R-carboxylethoxy)-4-aminomethylphenyl]aminocarbonylmethyl-1,3,4,5-tetrahydrobenz[c,d]indole-2-carboxylic acid hydrochloride monohydrate as a NMDA receptor antagonist.

RX(1) OF 1



(step 1)



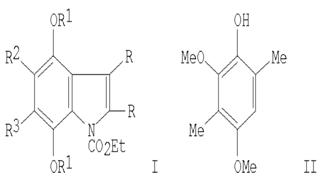
51%

NOTE: room temp. for 1 h; ice-temp. for 1 h

L20 ANSWER 5 OF 8 CASREACT COPYRIGHT 2009 ACS on STN

104:109408 Synthesis of 4,7-indolequinones. The oxidative demethylation of 4,7-dimethoxyindoles with ceric ammonium nitrate. Kitahara, Yoshiyasu; Nakahara, Shinsuke; Numata, Ryuichi; Kubo, Akinori (Meiji Coll. Pharm., Tokyo, 154, Japan). Chemical & Pharmaceutical Bulletin, 33(5), 2122-8 (English) 1985. CODEN: CPBTAL. ISSN: 0009-2363.

GI



AB The indoles I (R,R3 = H, Me; R1 = Me, Et, Ph; R2 = H, OMe) were synthesized by reductive cyclization of the appropriate dinitrostyrene or (nitrophenyl)acetaldehyde. The oxidative demethylations of I and phenol II with ceric ammonium nitrate yielded the corresponding 4,7-diones and p-quinone resp.

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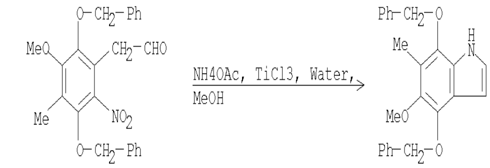
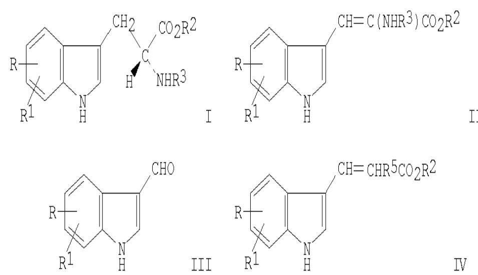
RX(28) OF 151



L20 ANSWER 6 OF 8 CASREACT COPYRIGHT 2009 ACS on STN

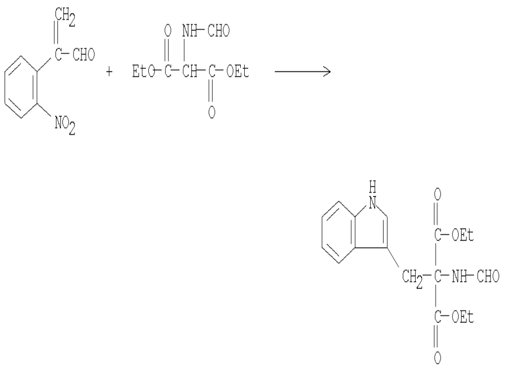
89:44226 Indole derivatives. Batcho, Andrew David; Hengartner, Urs Oskar; Leimgruber, Willy; Scott, John William; Valentine, Donald, Jr. (Hoffmann-La Roche, F., und Co. A.-G., Switz.). Ger. Offen. DE 2727671 19780105, 29 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1977-2727671 19770620.

GI



AB D-Tryptophans I (R and R1 = H, halo, OH, NH2, alkyl, alkoxy, aralkoxy, trihalomethyl; R2 = R3 = H) were prepared by asym. hydrogenating indoleacrylic acids II [R2 = alkyl, aryl; R3 = COR4 (R4 = H, alkyl, aryl, alkoxy, haloalkyl)] over a complex of a Rh compound and a chiral tertiary phosphine and hydrolyzing the resulting I [R2 = alkyl, aryl, ammonium, alkylammonium, R3 = COR4]. II were prepared by either condensing indolecarboxaldehydes III with an alkyl acylaminomalonate or by reducing the nitroacrylate IV (R5 = NO2, R2 = same as in II) and acylating the resulting amine. Thus, 6-chloroindole was treated with EtOCH:C(NO2)CO2Me to give II.HCl (R = 6-Cl, R1 = R3 = H, R2 = Me), which was acetylated and saponified to give II (R = 6-Cl, R1 = R2 = H, R3 = Ac). The latter was hydrogenated over [Rh(1,5-cyclooctadiene)(Cl)]2 and chiro-trans-4,5-bis(di-m-tolylphosphinomethyl)-2,2-dimethyl-1,3-dioxolane to give N-acetyl-6-chloro-D-tryptophan, which was hydrolyzed with 2N HBr to give 6-chloro-D-tryptophan.

RX(28) OF 69 - 2 STEPS



L20 ANSWER 7 OF 8 CASREACT COPYRIGHT 2009 ACS on STN

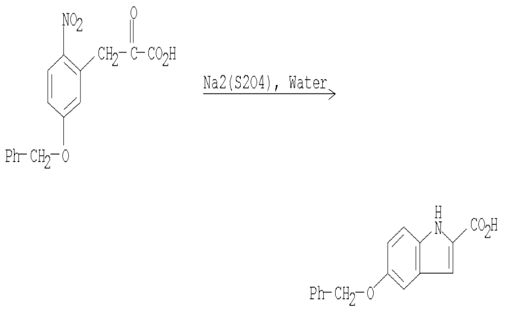
50:27880 Ergot alkaloids. XL. A new synthesis of bufotenine and related hydroxytryptamines. Stoll, A.; Troxler, F.; Peyer, J.; Hofmann, A. (Sandoz, Basel, Switz.). Helvetica Chimica Acta, 38, 1452-72 (German) 1955. CODEN: HCACAV. ISSN: 0018-019X.

AB cf. preceding abstract Nitrosation of m-MeC6H4OH and oxidation of the NO compound give 63% 2,5-(O2N)(HO)C6H3Me, m. 129-30°, which is converted into 87% 2,5-(O2N)(PhCH2O)C6H3Me (I). Treating I mole I with 2 mol (CO2Et)2 and 2 mol EtOK according to Burton and Stoves (C.A. 32, 550.1) at below 8° gives 87% 2-nitro-5-benzyloxyphenylpyruvic acid, m. 112-13°, which (55 g.), reductively cyclized in 600 cc. H2O and 80 cc. 2N NaOH with 70 g. Na2S2O4 added in small portions until the color reaction (deep red) with NaOH is neg. and acidified with dilute HCl, gives 48.5% 5-benzyloxyindole-2-carboxylic acid (II), m. 194-6°. Heating II in quinaldine with Cu powder at 245-50° gives 80% 5-benzyloxyindole (III), m. 103-5°, which, shaken in MeOH with Pd-asbestos (IV) and H, gives 5-hydroxyindole, long needles, m. 107-8°. Treating III in 1:1 EtOH-AcOH with Me2NH and CH2O according to Ek and Witkop (C.A. 49, 12437i) gives 84% 5-benzyloxygramine (V), m. 138°. Adding (20 min.) with stirring 420 cc. MeI to 30 g. V, keeping the mixture 15 h. at 5°, heating the methiodide with 60 g. NaCN in 1.1 l. H2O 2 h. at 80°, extracting the solution with CHCl3, evaporating the CHCl3, taking up the residue (29.6 g.) in 250 cc. Et2O, and diluting the concentrated Et2O solution with petr. ether give 85% 5-benzyloxy-3-indoleacetonitrile (VI), prisms, m. 75-8°. Refluxing 20 g. VI in 140 cc. EtOH and 100 cc. H2O 15 h. with 45 g. KOH, acidifying the mixture with 60 cc. AcOH, and diluting the filtered solution with 500 cc. H2O give 20.6 g. 5-benzyloxy-3-indoleacetic acid, m. 145-7°, which is converted with CH2N2 into the Me ester and the latter heated with N2H4 1.5 h. at 135°, giving 95% 5-benzyloxy-3-indoleacethydrazide (VII), leaflets, m. 153-4°. Adding dropwise 60 cc. N HCl to a mixture of 14.7 g. VII in 250 cc. dioxane and 50 cc. N NaNO2 solution, extracting the acetazide with Et2O, evaporating the Et2O, and treating the residual azide with 50 g. anhydrous Me2NH 3 h. at 5° give 60% 5-benzyloxy-3-indoleacetdimethylamide (VIII), platelets, m. 138-40°. In a similar way the following addnl. amides are prepared:

Me, short prisms, m. 141-2°; Et, prisms, m. 126-8°, di-Et, needles, m. 120-1°; H2NCH2CH2, plates, m. 137-9°; and piperidide, leaflets, m. 129-30°. Adding dropwise 1.26 g. LiAlH4 in 200 cc. Et2O in a N arm. to 3.65 g. VIII in 80 cc. THF, stirring the mixture 1 h. at 55°, and working it up in the usual way give 80% 5-benzyloxy-ω-N,N-dimethyltryptamine (bufotenine benzyl ether) (IX), pointed prisms, m. 87-9° [acid oxalate (X), fine leaflets, m. 177-8°]. Similar reduction of the corresponding amides gives the following N-substituted tryptamines: Me, plates, m. 84-6° [acid oxalate (XI), needles, m. 201-3°]; Et, crystals, m. 59-61° (acid oxalate, short needles, m. 187-9°) [the ω-N,N-diethyl homolog does not crystallize (acid oxalate, prisms, m. 162°)]; H2NCH2CH2, does not crystallize (bis-acid oxalate, leaflets, m. 221-2°); N-[β-(5-benzyloxy-3-indolyl)ethyl]piperidine, prisms, m. 136-8°. Shaking 3.45 g. IX in 75 cc. MeOH with 2 g. 5% IV and H 1.5 h. gives 78% bufotenine (XII), stout prisms, m. 138-40°. With FeCl3 in AcOH and concentrated H2SO4, XII gives a reddish color, turning to blue after 1-2 s. The UV absorption curves of XII in EtOH, 0.1N HCl, and 0.1N NaOH, and the IR absorption curves of XII and of natural XII are given. Shaking 1.85 g. X in 200 cc. MeOH with IV in H gives 86% XII acid oxalate, needles, m. 89-90°. Treating 1.1 g. XII in 2 cc. MeOH with 2 cc. MeI 3 h. at 20° gives 1.7 g. XII methiodide, stout prisms, m. 214-15°. Dissolving 2.9 g. XII and 2.3 g. creatinine sulfate (XIII) in 14 cc. N H2SO4 and 40 cc. boiling H2O and diluting the solution with Me2CO give a 5.3 g. XII-XIII complex, fine needles, m. 147-9°. Debenzylation of XI gives 5-hydroxy-ω-N-methyltryptamine (ω-N-methylserotonin), short pointed prisms and plates, m. 153-6°; N-Et homolog, short prisms, m. 239-40°; N,N-di-Et homolog, polyhedrons and prisms, m. 147-9° (oxalate, m. 230-2°); N-H2NCH2CH2 analog, bis-acid oxalate, leaflets, m. 208-9°; N-[β-(5-hydroxy-3-indolyl)ethyl]piperidine, stout prisms, m. 201-3° (oxalate, pointed prisms, m. 243-7°). Refluxing 30.6 g. 2,6-O2N(HO)C6H3Me in 150 cc. EtOH containing 4.6 g. Na 8 h. with 25.4 g. PhCH2Cl, adding H2O, distilling off the EtOH in vacuo, and extracting with Et2O give 63.8% 2,6-O2N(PhCH2O)C6H3Me (XIV), b0.8 170-6°, m. 65-6°. Condensation of XIV with (CO2Et)2 in the presence of EtOK gives the 2-nitro-6-benzyloxyphenylpyruvic acid which is directly converted into 64% (overall) 4-benzyloxy-2-indolecarboxylic acid (XV) (purified via its Na salt), m. 241-2°. Decarboxylation of XV in quinaldine in the presence of Cu powder gives 62% 4-benzyloxyindole (XVI), needles, m. 72-4°, which, treated in MeOH with H in the presence of IV, gives 4-hydroxyindole, hexagonal plates, m. 97-9°. Treating XVI with Me2NH in the same way as in the preparation of V gives 89% 4-benzyloxygramine (XVII), hexagonal leaflets, m. 94-8°. Treating the methiodide of XVII with NaCN gives 60% 4-benzyloxy-3-indoleacetonitrile, m. 97-100°, which, reduced with LiAlH4, gives 81% 4-benzyloxytryptamine, plates, m. 117-20° [acid oxalate (XVIII), hexagonal plates, m. 188-9°]. Shaking 3.3 g. XVIII in 270 cc. MeOH with Pd and H gives 4-hydroxytryptamine (XIX) oxalate, clusters of platelets, m. 269-70°; free base does not crystallize. XIX-XIII complex, needles, m. 250-5°. Condensation of 121.5 g. 2,4-O2N(PhCH2O)C6H3Me with (CO2Et)2 gives 91% 2-nitro-4-benzyloxyphenylpyruvic acid, m. 133-5° (B. and S. (loc. cit.) found 89-90°), which is converted into 51% 6-benzyloxy-2-indolecarboxylic acid (XX), m. 199-200° (decomposition). Decarboxylation of XX gives 46% 6-benzyloxyindole, leaflets, m. 118-20°, which, with Pd and H in MeOH, gives 6-hydroxyindole (XXI),

hexagonal leaflets, m. 124-6°. XXI is converted into 80% 6-benzyloxygramine (XXII), long rods, m. 136-8°. Converting XXII into the methiodide and treating the latter with NaCN give 75% 6-benzyloxy-3-indoleacetonitrile, leaflets, m. 136-7°, which, reduced with LiAlH4 in THF, gives 71% 6-benzyloxytryptamine (XXIII), fine needles, m. 92-6° (oxalate, shiny leaflets, m. 260-5°). XXIII, debenzylated with Pd and H, gives 6-hydroxytryptamine (XXIV) which does not crystallize. XXIII is converted into its sulfate and the latter (1.4 g.) is shaken in 500 cc. H2O with 500 mg. IV and H, the filtrate concentrated to 100 cc., and 0.72 g. XIII added, giving 85% XXIV-XIII complex, fine needles, m. 212-15°. The UV and IR absorption maximum of some of the compds. are given.

RX(1) OF 3



49%

NOTE: Classification: Isomerisation; Reductive coupling; Cyclisation; Heterocycle formation; # Conditions: Na2S2O4 NaOH; H2O

L20 ANSWER 8 OF 8 CASREACT COPYRIGHT 2009 ACS on STN

43:8352 Chemistry of bacteria. I. Synthesis of hydroxyindoles. Beer, R. J. S.; Clarke, Kenneth; Khorana, H. G.; Robertson, Alexander Journal of the Chemical Society 1605-9 (Unavailable) 1948. CODEN: JCSOA9. ISSN: 0368-1769.

AB Indoles hydroxylated in the C6H6 nucleus are needed to identify 2 isomeric products (C8H7ON) obtained in the degradation of violacein (from Chromobacterium violaceum). 2,5-O2N(HO)C6H3CHO (5 g.), 6 g. aceturic acid, 6 g. AcONa, and 15 mL. Ac2O, heated 1.5 h. on the steam bath, the mixture kept 10 h., and diluted with 10 mL. MeOH and 5 mL. H2O, give 5-keto-2-methyl-4-(2-nitro-5-acetoxybenzylidene)-4,5-dihydrooxazole, yellow, m. 140°, and the hydroxybenzylidene analog, m. 173°; addition of 20 mL. concentrated H2SO4 to 25 mL. H2O containing 4 g. of the mixed azlactones and boiling 1 min. give 3.2 g. (2-nitro-5-hydroxyphenyl)pyruvic acid (I), m. 194° (decomposition); I also results on boiling the azlactones 4-5 h. with 1.5 N HCl; oxime, m. 181°. I (5 g.) in 34 mL. NH4OH (d. 0.88) and 14 mL. H2O, treated with 44 g. FeSO4 in 48 mL. H2O and the mixture refluxed 1.5 h., gives 3 g. 5-hydroxy-2-indolecarboxylic acid (II), m. 246° (decomposition); decarboxylation of 0.5 g. II in 5 mL. C3H5(OH)3 at 225-30° (25 min.) gives a poor yield of 5-hydroxyindole (picrate, orange-red, m. 167°); other conditions did not give better results. 2,4-O2N(PhCH2O)C6H3COCO2H (oxime, m.

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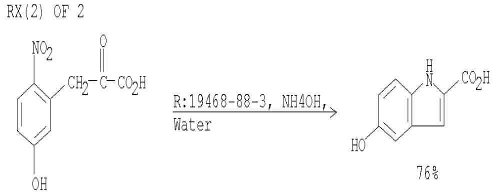
182° (decomposition)) yields 6-(benzyloxy)-2-indolecarboxylic acid, m. 200° (decomposition), debenzylation of which (2 g. and 2 g. 10% Pd-C in 100 mL. AcOH) gives 0.9 g. 6-hydroxy-2-indolecarboxylic acid (III), m. 236° (decomposition); 0.5 g. III in C3H5(OH)3, heated 20 min. at 220-30°, gives 0.2 g. 6-hydroxyindole m. 125.5° (picrate, dark red, m. 154-6° (decomposition)). 2,3-O2N(HO)C6H3Me (5 g.), 3.8 mL. PhCH2Br, and excess K2CO3 in 100 mL. boiling Me2CO (2.5 h.) give 6.5 g. 2-nitro-3-(benzyloxy)toluene, m. 36°; condensation of 24 g. with 15 g. (CO2Et)2 with EtOK gives 15.5 g. 2-nitro-3-(benzyloxy)phenylpyruvic acid (IV), yellow, m. 125° (oxime, m. 190-1°). Reduction and cyclization of 3.8 g. IV give 2.2 g. 7-(benzyloxy)-2-indolecarboxylic acid (V), m. 164°; debenzylation of 2 g. V gives 1 g. 7-hydroxy-2-indolecarboxylic acid, m. 252°; decarboxylation of 0.5 g. yields 20 mg. 7-hydroxyindole, m. 96°. 2,6-O2N(HO)C6H3CHO (1 g.) and 0.4 g. MeNO2 in EtOH at -10°, treated with 0.7 g. KOH in 10 mL. EtOH, the mixture carefully acidified with cooled HCl, and the yellow oil (obtained by extraction with ether) gently warmed (15 min.) with 2 g. AcONa and 3 mL. Ac2O, give 1.35 g. β,2-dinitro-6-acetoxystyrene (VI), light tan, m. 128-30°. Reaction of 0.5 g. VI, 2 g. Fe, 4 mL. EtOH, and 4 mL. AcOH, gently refluxed 10-12 min., gives 0.1-0.12 g. 4-acetoxyindole (VII), m. 100°; 0.1 g. VII in 3 mL. MeOH saturated at 0° with NH3 and the solution kept 16 h. below 5°, gives 70-80% 4-hydroxyindole, m. 98° (picrate, red, becomes partly yellow at 150° and chars at 180°); it gives a dark blue color with alc. FeCl3 and a red color and strong green fluorescence with Ehrlich reagent in the cold. 2,5-O2N(HO)C6H3CHO yields β,2-dinitro-5-acetoxystyrene, straw, m. 118-19°; this yields 50-5% 5-acetoxyindole, m. 113-14°, which gives 5-hydroxyindole. 5,2-O2N(HO)C6H3CHO (1 g.) and EtNO2 give 0.7 g. β,2-dinitro-5-acetoxy-β-methylstyrene, pale brown, m. 88-9°; reduction with Fe and AcOH gives 5-acetoxy-2-methylindole, m. 128-30°, which yields 80% 5-hydroxy-2-methylindole, m. 133-4°, gives a brownish purple color with alc. FeCl3 and a very intense red color with Ehrlich reagent (picrate, red, m. 157-8° (decomposition)). 6,2-O2N(HO)C6H3CHO (1 g.), 0.8 g. aceturic acid, 0.8 g. AcONa, and 3 mL. Ac2O, heated 1 h. on the steam bath, give 1.3 g. 5-keto-4-(2-nitro-6-acetoxybenzylidene)-2-methyl-4,5-dihydrooxazole, yellow, m. 180°; hydrolysis of 1 g. with 1.5 N HCl (6 h. on the steam bath) gives 0.49 g. 5-nitro-3-hydroxycoumarin, yellow, m. 206-7° (2,4-dinitrophenylhydrazone, orange, m. above 250°). 6-Nitro-2-(benzyloxy)toluene, m. 62°. 2,6-O2N(HO)C6H3CHO (1 g.), 0.5 mL. AcOH, 0.5 g. AcONH4, and 5 mL. EtOH gradually deposit 0.85 g. 2-(2-nitro-6-hydroxyphenyl)-5-nitro-1,3,2H-benzoxazine, orange-yellow, m. 204-5°; alc. FeCl3 gives an orange color slowly changing to red; acetate, m. 164°. The stability of the various hydroxyindoles is discussed.

RX(2) OF 2



76%

NOTE: Classification: Isomerisation; Reductive coupling; Cyclisation; Heterocycle formation; # Conditions: FeSO4 NH4OH; H2O ; Rf 1h30mn

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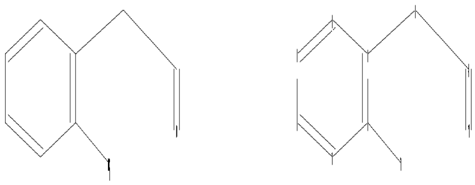

chain nodes :
7 8 9
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
10
chain bonds :
5-8 6-7 8-9 9-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
9-10
exact bonds :
5-8 6-7 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

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SEARCH TIME: 00.00.01

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                        BATCH   **COMPLETE**
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PROJECTED ANSWERS: 7023 TO   9457

L22   50 SEA SSS SAM L21

L23   14 L22

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SEARCH TIME: 00.00.01

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PROJECTED ANSWERS:           7023 TO     9457

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L3         114 S L1 FULL
L4           0 S L3 AND CARBON MONOXIDE
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L14          3 S L11 AND IRON
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               S L21

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To search a role for a specific substance, append the CAS Registry Number or a Registry File L-number answer set with a slash and the code for the role, e.g., 67-68-5/THU. To search more than one role,

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The following is a hierarchical list of CAS roles. Under each super role are listed the specific roles that generate the super role.

List of CAS Roles (1)

ANST Analytical Study

ANT Analyte
AMX Analytical Matrix
ARG Analytical Reagent Use
ARU Analytical Role, Unclassified

BIOL Biological Study

ADV Adverse Effect, Including Toxicity
AGR Agricultural Use
BAC Biological Activity or Effector, Except Adverse (2)
BCP Biochemical Process (3)
BMF Bioindustrial Manufacture
BOC Biological Occurrence (2)
BPN Biosynthetic Preparation
BPR Biological Process (2)
BSU Biological Study, Unclassified
BUU Biological Use, Unclassified
COS Cosmetic Use (3)
DGN Diagnostic Use (3)
DMA Drug Mechanism of Action (3)
FFD Food or Feed Use
MFM Metabolic Formation (2)
NPO Natural Product Occurrence (3)
PAC Pharmacological Activity (3)
PKT Pharmacokinetics (3)
THU Therapeutic Use

CMBI Combinatorial Study (3)

CPN Combinatorial Preparation (3)

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CRT Combinatorial Reactant (3)
CRG Combinatorial Reagent (3)
CST Combinatorial Study (3)
CUS Combinatorial Use (3)

FORM Formation, Nonpreparative

FMU Formation, Unclassified
GFM Geological or Astronomical Formation
MFM Metabolic Formation (2)

OCCU Occurrence

BOC Biological Occurrence (2)
GOC Geological or Astronomical Occurrence
NPO Natural Product Occurrence (3)
OCU Occurrence, Unclassified
POL Pollutant

PREP Preparation (4)

BMF Bioindustrial Manufacture
BPN Biosynthetic Preparation
BYP Byproduct
CPN Combinatorial Preparation (3)
IMF Industrial Manufacture
PUR Purification or Recovery
PNU Preparation, Unclassified (5)
SPN Synthetic Preparation

PROC Process

BCP Biochemical Process (3)
BPR Biological Process (2)
GPR Geological or Astronomical Process
PEP Physical, Engineering, or Chemical Process
CPS Chemical Process (6)
EPR Engineering Process (6)
PYP Physical Process (6)
REM Removal or Disposal

PRPH Prophetic Substance (7)

RACT Reactant or Reagent (2,6)

RCT Reactant (8)
 CRT Combinatorial Reactant (3)
RGT Reagent (3)
 CRG Combinatorial Reagent (3)

USES Uses

AGR Agricultural Use
ARG Analytical Reagent Use
BUU Biological Use, Unclassified
CAT Catalyst Use
COS Cosmetic Use (3)

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 CUS   Combinatorial Use (3)
 DGN   Diagnostic Use (3)
 FFD   Food or Feed Use
 MOA   Modifier or Additive Use
 NUU   Other Use, Unclassified (9)
 POF   Polymer in Formulation
 TEM   Technical or Engineered Material Use
 THU   Therapeutic Use

 Specific roles that are not uppposted to any super roles:

 MSC   Miscellaneous
 PRP   Properties

 (1)  Super roles have 4-letter codes. Specific roles have 3-letter
      codes.  Under each super role are listed the corresponding
      specific roles that are retrieved when you search that
      super role.
 (2)  Used from CA Vol. 66 (1967) to Vol. 135 (2001)
 (3)  Used starting with CA Vol. 136 (2002)
 (4)  The PREP super role has been added to records back to 1907.
 (5)  Used from CA vol. 66 (1967) to vol. 145 (2006).
 (6)  Used from CA vol. 136 (2002) to CA vol. 145 (2006).
 (7)  Used starting with records from CA vol. 148 (2008).
 (8)  Searching the RCT (Reactant) role retrieves references from CA
      Vol. 66 (1967) to the present.  Searching the RACT (Reactant or
      Reagent) super role retrieves references with the CRT, CRG, RGT,
      or RCT references starting with CA Vol. 136 (2002).
 (9)  Starting with CA Vol. 136 (2002), the searchable text for the
      NUU role changed from NONBIOLOGICAL USE, UNCLASSIFIED/RL to
      OTHER USE, UNCLASSIFIED/RL. Search the code NUU/RL to retrieve
      records from CA Vol. 66 (1967) to the present.


=> d his

     (FILE 'HOME' ENTERED AT 11:15:49 ON 16 MAR 2009)

     FILE 'CASREACT' ENTERED AT 11:16:04 ON 16 MAR 2009
L1                STRUCTURE UPLOADED
L2              3 S L1
L3            114 S L1 FULL
L4              0 S L3 AND CARBON MONOXIDE
L5           5849 S CARBON MONOXIDE

     FILE 'REGISTRY' ENTERED AT 11:17:25 ON 16 MAR 2009
L6              1 S CARBON MONOXIDE/CN

     FILE 'CASREACT' ENTERED AT 11:17:52 ON 16 MAR 2009
L7          10878 S 630-08-0
L8              2 S L7 AND L3
L9                STRUCTURE UPLOADED
L10             6 S L9
L11           151 S L9 FULL
L12             3 S L11 AND L7
L13             1 S L12 NOT L8
L14             3 S L11 AND IRON
L15             3 S L11 AND CARBONYL
L16             2 S L11 AND COMPLEX
```

Print selected from 10562215.trn

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L17             9 S L13-L16
L18             8 S L14-L16
L19             8 S L18 NOT L12
L20             8 S L18 NOT L8
L21               STRUCTURE UPLOADED

     FILE 'CAPLUS' ENTERED AT 11:33:50 ON 16 MAR 2009
                  S L21

     FILE 'REGISTRY' ENTERED AT 11:33:53 ON 16 MAR 2009
L22            50 S L21

     FILE 'CAPLUS' ENTERED AT 11:33:54 ON 16 MAR 2009
L23            14 S L22

     FILE 'REGISTRY' ENTERED AT 11:33:58 ON 16 MAR 2009
L24            50 S L21
L25          8317 S L21 FULL

     FILE 'CAPLUS' ENTERED AT 11:34:26 ON 16 MAR 2009

=> s l25/ract
          2918 L25
       3247332 RACT/RL
L26       1497 L25/RACT
                 (L25 (L) RACT/RL)

=> s l26 and carbon monoxide
       1444457 CARBON
         30213 CARBONS
       1455082 CARBON
                 (CARBON OR CARBONS)
        201108 MONOXIDE
          1090 MONOXIDES
        201684 MONOXIDE
                 (MONOXIDE OR MONOXIDES)
        170555 CARBON MONOXIDE
                 (CARBON(W)MONOXIDE)
L27          5 L26 AND CARBON MONOXIDE

=> d cbib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 5 ANSWERS - CONTINUE? Y/(N):y

L27  ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2009 ACS on STN
2008:994205   Document No. 149:3066210  Iodomethane.  Sulikowski, Gary A.;
     Sulikowski, Michelle M.; Haukaas, Michael H.; Moon, Bongjin (USA).  e-EROS
     Encyclopedia of Reagents for Organic Synthesis, No pp. given.  John Wiley
     & Sons, Ltd.: Chichester, UK. (English) 2001.  CODEN: 69KUHI.  OTHER
     SOURCES: CASREACT 149:306621.
AB   A review of the article Iodomethane.
IT   4212-33-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (Iodomethane)
RN   4212-33-3  CAPLUS
CN   Ethanone, 2-(2-nitrophenyl)-1-phenyl-  (CA INDEX NAME)
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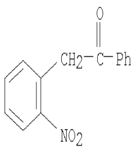
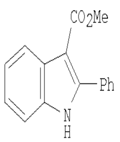
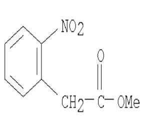


L27 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
2008:510694 Document No. 149:794360 Palladium-catalyzed synthesis of 3-indolecarboxylic acid derivatives. Soderberg, Bjorn C. G.; Banini, Serge R.; Turner, Michael R.; Minter, Aaron R.; Arrington, Amanda K. (C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV, 26506-6045, USA). Synthesis (6), 903-912 (English) 2008. CODEN: SYNTBF. ISSN: 0039-7881. OTHER SOURCES: CASREACT 149:79436. Publisher: Georg Thieme Verlag.
GI


I

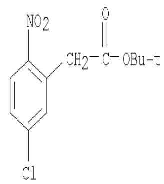
AB Indoles having an ester functionality in the 3-position, e.g., I, were prepared from 2-(2-nitrophenyl)propenoic acid derivs. via a palladium-catalyzed reductive N-heteroannulation using carbon monoxide as the ultimate reducing agent. The starting materials were prepared either by a Stille coupling of 2-halo-1-nitrobenzenes with Et 2-(tributylstannyl)-2-propenoate or by vicarious nucleophilic substitution of nitrobenzenes followed by a Knoevenagel-type condensation with an aldehyde. Synthesis of an example of a 3-nitrile- and a 3-sulfone-substituted indole is also described using the same type of methodologies.
IT 30095-98-8 81327-28-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (aza)indole carboxylates/sulfone/nitrile via palladium/phenanthroline (or tri-Ph phosphine) catalyzed reductive N-heteroannulation of α,β-unsatd. ester/sulfone/nitrile intermediates)
RN 30095-98-8 CAPLUS
CN Benzeneacetic acid, 2-nitro-, methyl ester (CA INDEX NAME)



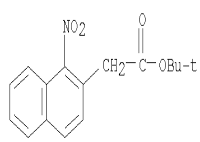
RN 81327-28-8 CAPLUS

Print selected from 10562215.trn

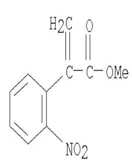
CN Benzeneacetic acid, 5-chloro-2-nitro-, 1,1-dimethylethyl ester (CA INDEX NAME)



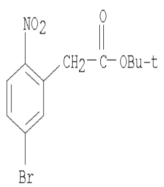
IT 344449-11-2P 494836-60-1P 878672-60-7P
1033265-16-5P 1033265-29-0P 1033265-31-4P
1033265-33-6P 1033265-35-8P 1033265-37-0P
1033265-39-2P 1033265-41-6P 1033265-69-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (aza)indole carboxylates/sulfone/nitrile via palladium/phenanthroline (or tri-Ph phosphine) catalyzed reductive N-heteroannulation of α,β-unsatd. ester/sulfone/nitrile intermediates)
RN 344449-11-2 CAPLUS
CN 2-Naphthaleneacetic acid, 1-nitro-, 1,1-dimethylethyl ester (CA INDEX NAME)



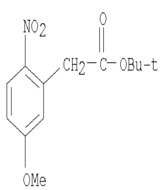
RN 494836-60-1 CAPLUS
CN Benzeneacetic acid, α-methylene-2-nitro-, methyl ester (CA INDEX NAME)



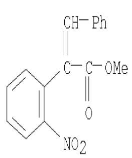
RN 878672-60-7 CAPLUS
CN Benzeneacetic acid, 5-bromo-2-nitro-, 1,1-dimethylethyl ester (CA INDEX NAME)



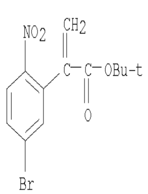
RN 1033265-16-5 CAPLUS
CN Benzeneacetic acid, 5-methoxy-2-nitro-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 1033265-29-0 CAPLUS
CN Benzeneacetic acid, 2-nitro-α-(phenylmethylene)-, methyl ester (CA INDEX NAME)

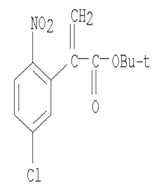


RN 1033265-31-4 CAPLUS
CN Benzeneacetic acid, 5-bromo-α-methylene-2-nitro-, 1,1-dimethylethyl ester (CA INDEX NAME)

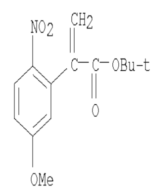


RN 1033265-33-6 CAPLUS
CN Benzeneacetic acid, 5-chloro-α-methylene-2-nitro-, 1,1-dimethylethyl

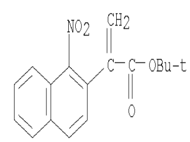
ester (CA INDEX NAME)



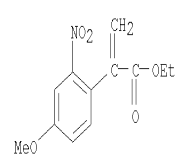
RN 1033265-35-8 CAPLUS
CN Benzeneacetic acid, 5-methoxy-α-methylene-2-nitro-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 1033265-37-0 CAPLUS
CN 2-Naphthaleneacetic acid, α-methylene-1-nitro-, 1,1-dimethylethyl ester (CA INDEX NAME)

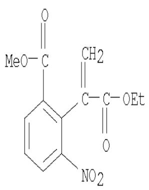


RN 1033265-39-2 CAPLUS
CN Benzeneacetic acid, 4-methoxy-α-methylene-2-nitro-, ethyl ester (CA INDEX NAME)



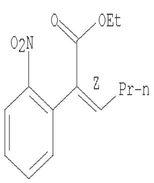
RN 1033265-41-6 CAPLUS

CN Benzeneacetic acid, 2-(methoxycarbonyl)-α-methylene-6-nitro-, ethyl
ester (CA INDEX NAME)

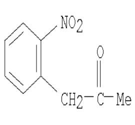


RN 1033265-69-8 CAPLUS
CN Benzeneacetic acid, α-butylidene-2-nitro-, ethyl ester, (αZ)-
(CA INDEX NAME)

Double bond geometry as shown.



L27 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
2007:404312 Document No. 146:462149 Development of novel catalytic reactions of heterocyclic compounds toward new pesticide development. Tanaka, Norio (Electr. Mater. Res. Lab., Nissan Chemical Industries, Ltd., Japan). Farumashia, 43(3), 231-235 (Japanese) 2007. CODEN: FARUAW. ISSN: 0014-8601. Publisher: Pharmaceutical Society of Japan.
AB A review on catalytic reactions of N-containing heterocyclic compds. for the development of pesticides by Nissan Chemical Industries, Ltd., Japan: (1) preparation of pyrazolecarboxylic acids by liquid-phase oxidation using Co Mn bromide catalysts, (2) N-alkylation of azoles with alcs. using Ru catalysts, (3) preparation of indoles by reductive cyclization of (E)-β-nitrostyrenes or o-nitrophenylacetones using transition metal catalysts in CO atmospheric
IT 1969-72-8D, o-Nitrophenylacetone, derivs.
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of indoles by reductive cyclization of nitrostyrenes or nitrophenylacetones using transition metal catalysts in CO atmospheric)
RN 1969-72-8 CAPLUS
CN 2-Propanone, 1-(2-nitrophenyl)- (CA INDEX NAME)



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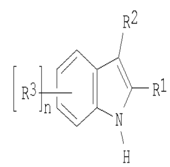
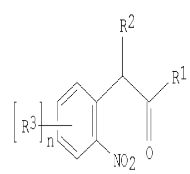
L27 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
2005:14373 Document No. 142:936770 Process for the preparation of indoles via reductive cyclization. Sakurai, Yasuhiro; Utsunomiya, Tomohisa; Tanaka, Norio (Nissan Chemical Industries, Ltd., Japan). PCT Int. Appl. WO 2005000812 A1 20050106, 31 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2004-JP9001 20040625. PRIORITY: JP 2003-184359 20030627.
GI



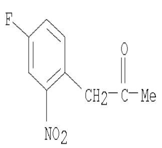
I



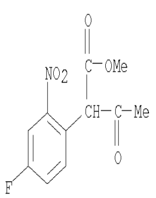
II

AB A process for the preparation of indoles I [R1, R2 = H, (un)substituted alkyl, etc.; R3 = (un)substituted alkyl, etc.; n = 0-4] from 2-nitrobenzyl ketone compds. II [R1, R2 = H, (un)substituted alkyl, etc.; R3 = (un)substituted alkyl, etc.; n = 0-4] in the presence of a catalyst comprising a group VIII metal of the periodic table was provided. For example, in a stainless autoclave, a mixture of 4-fluoro-2-nitrophenylacetone (1.0 g), cyclopentadienylirondicarbonyl dimer (72 mg), toluene (40.0 g) and carbon monoxide (50 kgf/cm2) at 120 °C for 5 h, afforded 6-fluoro-2-methylindole (0.64 g, 95.0% yield), analyzed by liquid chromatog. The process enables an indole compound to be selectively produced in high yield from a 2-nitrobenzylcarbonyl compound, and hardly yields an indoline compound as a reduction byproduct, this byproduct generation having been a problem in the catalytic hydrogenation method employing a noble-metal catalyst. The indole derivative produced by the process is useful as an intermediate for various fine chems. such as medicines and agricultural chems.

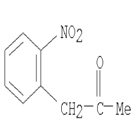
IT 39616-99-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation of 1-(4-fluoro-2-nitrophenyl)acetone via decarboxylation)
RN 39616-99-4 CAPLUS
CN 2-Propanone, 1-(4-fluoro-2-nitrophenyl)- (CA INDEX NAME)



IT 816450-30-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation of 2-(2-nitrophenyl)-3-oxobutanoic acid Me eater derivative via nucleophilic substitution of 2,5-difluoronitrobenzene with Et acetoacetate)
RN 816450-30-3 CAPLUS
CN Benzeneacetic acid, α-acetyl-4-fluoro-2-nitro-, methyl ester (CA INDEX NAME)



IT 1969-72-8 6127-15-7 57330-58-2
81327-26-6 85355-52-8 606092-02-8
816450-35-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of indole derivative from 2-nitrobenzyl ketone compds. using group
VIII metal catalysts.)
RN 1969-72-8 CAPLUS
CN 2-Propanone, 1-(2-nitrophenyl)- (CA INDEX NAME)



RN 6127-15-7 CAPLUS
CN 2-Propanone, 1-(4-bromo-2-nitrophenyl)- (CA INDEX NAME)

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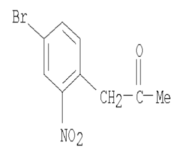
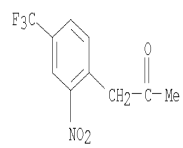
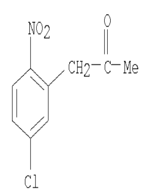


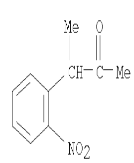
RN 57330-58-2 CAPLUS
CN 2-Propanone, 1-[2-nitro-4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



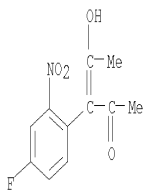
RN 81327-26-6 CAPLUS
CN 2-Propanone, 1-(5-chloro-2-nitrophenyl)- (CA INDEX NAME)



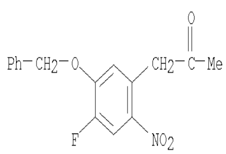
RN 85355-52-8 CAPLUS
CN 2-Butanone, 3-(2-nitrophenyl)- (CA INDEX NAME)



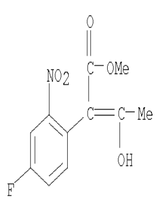
RN 606092-02-8 CAPLUS
CN 3-Penten-2-one, 3-(4-fluoro-2-nitrophenyl)-4-hydroxy- (CA INDEX NAME)



RN   816450-35-8 CAPLUS
CN   2-Propanone, 1-[4-fluoro-2-nitro-5-(phenylmethoxy)phenyl]- (CA INDEX
     NAME)

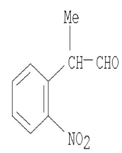


IT   606092-03-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
     RACT (Reactant or reagent)
        (preparation of indole derivative from 2-nitrobenzyl ketone compds. using
group
        VIII metal catalysts.)
RN   606092-03-9 CAPLUS
CN   Benzeneacetic acid, 4-fluoro-α-(1-hydroxyethylidene)-2-nitro-,
     methyl ester (CA INDEX NAME)



L27 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
1981:442811   Document No. 95:428110 Original Reference No. 95:7321a,7324a
     Catalytic synthesis of 3-substituted indoles using carbon
     monoxide as building block and supported rhodium as catalyst.
     Ucciani, Eugene; Bonfand, Andre (Lab. Chim. Org. Appl., Fac. Sci. Tech.,
     Marseille, 13397/13, Fr.). Journal of the Chemical Society, Chemical
     Communications (3), 82-3 (English) 1981. CODEN: JCCCAT. ISSN: 0022-4936.
     OTHER SOURCES: CASREACT 95:42811.
AB   Skatole was prepared (.apprx.70%) from 2-O2NC6H4CH:CH2, under
     hydroformylation conditions, (CO, H, 160°) using C-supported Rh as
     a catalyst, via 2-O2NC6H4CMeCHO formation by homogeneous catalysis, reduction

     of the NO2 group by hetereogeneous catalysis, cyclization and thermal
     dehydration.
IT   78266-67-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
     RACT (Reactant or reagent)
        (preparation and reduction of, rhodium-catalyzed)
RN   78266-67-8 CAPLUS
CN   Benzeneacetaldehyde, α-methyl-2-nitro- (CA INDEX NAME)



=> s uccuiani/au
L28   0 UCCUIANI/AU

=> s ucciani ?/au
L29   318 UCCIANI ?/AU

=> s l19 and rhodium
             8 L19
         78733 RHODIUM
            33 RHODIUMS
         78735 RHODIUM
                 (RHODIUM OR RHODIUMS)
L30   1 L19 AND RHODIUM

=> s bonfand/au
L31   0 BONFAND/AU

=> s bonfand ?/au
L32   33 BONFAND ?/AU

=> s l32 and rhodium
         78733 RHODIUM
            33 RHODIUMS
         78735 RHODIUM
                 (RHODIUM OR RHODIUMS)
L33   2 L32 AND RHODIUM

=> s l33 nod l27
MISSING OPERATOR L33 NOD
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s l33 not l27
L34   1 L33 NOT L27

=> d cbib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y

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L34  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2009 ACS on STN
1991:494766   Document No. 115:94766  Original Reference No. 115:16301a,16304a
     Hydroformylation of fatty acid vinyl esters.  Bonfand, A.;
     Ucciani, E.; Luciani, A.; Sambuc, E. (Lab. Chim. Org. Appl., CNRS, Fr.).
     Revue Francaise des Corps Gras, 37(9-10), 281-7 (French) 1990.  CODEN:
     RFCGAE.  ISSN: 0035-3000.
AB   Hydroformylation of vinyl esters of lauric, myristic, palmitic, and
     stearic acids to obtain fatty esters of propanediol was investigated.  Of
     several catalytic systems tested, Rh/C was the most efficient, leading to
     aldesters instead of alc. esters.  Catalytic hydroformylation by Rh/C gave
     only one aldester, RCOOCH(CH3)CHO.  Reduction by NaBH4 yielded 2 alc. esters,
     RCOOCH(CH3)CH2OH (minor product) and RCOOCH2CH(CH3)OH (major product),
     regardless of the vinyl ester used.


=> d his

     (FILE 'HOME' ENTERED AT 11:15:49 ON 16 MAR 2009)

     FILE 'CASREACT' ENTERED AT 11:16:04 ON 16 MAR 2009
L1              STRUCTURE UPLOADED
L2            3 S L1
L3          114 S L1 FULL
L4            0 S L3 AND CARBON MONOXIDE
L5         5849 S CARBON MONOXIDE

     FILE 'REGISTRY' ENTERED AT 11:17:25 ON 16 MAR 2009
L6            1 S CARBON MONOXIDE/CN

     FILE 'CASREACT' ENTERED AT 11:17:52 ON 16 MAR 2009
L7        10878 S 630-08-0
L8            2 S L7 AND L3
L9              STRUCTURE UPLOADED
L10           6 S L9
L11         151 S L9 FULL
L12           3 S L11 AND L7
L13           1 S L12 NOT L8
L14           3 S L11 AND IRON
L15           3 S L11 AND CARBONYL
L16           2 S L11 AND COMPLEX
L17           9 S L13-L16
L18           8 S L14-L16
L19           8 S L18 NOT L12
L20           8 S L18 NOT L8
L21             STRUCTURE UPLOADED

     FILE 'CAPLUS' ENTERED AT 11:33:50 ON 16 MAR 2009
                S L21

     FILE 'REGISTRY' ENTERED AT 11:33:53 ON 16 MAR 2009
L22          50 S L21

     FILE 'CAPLUS' ENTERED AT 11:33:54 ON 16 MAR 2009
L23          14 S L22

     FILE 'REGISTRY' ENTERED AT 11:33:58 ON 16 MAR 2009
L24          50 S L21
L25        8317 S L21 FULL
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     FILE 'CAPLUS' ENTERED AT 11:34:26 ON 16 MAR 2009
L26        1497 S L25/RACT
L27           5 S L26 AND CARBON MONOXIDE
L28           0 S UCCUIANI/AU
L29         318 S UCCIANI ?/AU
L30           1 S L19 AND RHODIUM
L31           0 S BONFAND/AU
L32          33 S BONFAND ?/AU
L33           2 S L32 AND RHODIUM
L34           1 S L33 NOT L27

=> s 630-08-0/rn
        159419 630-08-0
           863 630-08-0D
L35     158661 630-08-0/RN
                 (630-08-0 (NOTL) 630-08-0D )

=> s l35 and l26
L36           4 L35 AND L26

=> d his
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     (FILE 'HOME' ENTERED AT 11:15:49 ON 16 MAR 2009)

     FILE 'CASREACT' ENTERED AT 11:16:04 ON 16 MAR 2009
L1              STRUCTURE UPLOADED
L2            3 S L1
L3          114 S L1 FULL
L4            0 S L3 AND CARBON MONOXIDE
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L17           9 S L13-L16
L18           8 S L14-L16
L19           8 S L18 NOT L12
L20           8 S L18 NOT L8
L21             STRUCTURE UPLOADED

     FILE 'CAPLUS' ENTERED AT 11:33:50 ON 16 MAR 2009
                S L21

     FILE 'REGISTRY' ENTERED AT 11:33:53 ON 16 MAR 2009
L22          50 S L21

     FILE 'CAPLUS' ENTERED AT 11:33:54 ON 16 MAR 2009
L23          14 S L22
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     FILE 'REGISTRY' ENTERED AT 11:33:58 ON 16 MAR 2009
L24         50 S L21
L25       8317 S L21 FULL

     FILE 'CAPLUS' ENTERED AT 11:34:26 ON 16 MAR 2009
L26       1497 S L25/RACT
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L33          2 S L32 AND RHODIUM
L34          1 S L33 NOT L27
L35     158661 S 630-08-0/RN
L36          4 S L35 AND L26

=> s l36 not l27
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